

On the Schmidt-rank-three bipartite and multipartite unitary operator

Lin Chen¹ and Li Yu¹

¹ Singapore University of Technology and Design, 20 Dover Drive, Singapore 138682

Unitary operations are physically implementable. We further the understanding of such operations by studying the possible forms of nonlocal unitary operators, which are bipartite or multipartite unitary operators that are not tensor product operators. They are of broad relevance in quantum information processing. We prove that any nonlocal unitary operator of Schmidt rank three on a $d_A \times d_B$ bipartite system is locally equivalent to a controlled unitary. This operator can be locally implemented assisted by a maximally entangled state of Schmidt rank $\min\{d_A^2, d_B\}$ when $d_A \leq d_B$. We further show that any multipartite unitary operator U of Schmidt rank three can be controlled by one system or collectively controlled by two systems, regardless of the number of systems of U . In the scenario of n -qubit, we construct non-controlled U for any odd $n \geq 5$, and prove that U is a controlled unitary for any even $n \geq 4$.

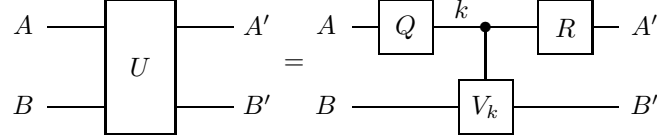
PACS numbers: 03.65.Ud, 03.67.Mn

I. INTRODUCTION

Bipartite and multipartite unitary operators play a fundamental role in quantum information processing. They are used to create quantum states, nonlocal correlations such as entanglement and discord [1], and to implement quantum circuits and computation. It is thus desirable to systematically implement multipartite unitary operators and understand their properties. So far this is a hard problem. The understanding of the forms and implementation schemes of multipartite unitary operators is still far from complete. For a survey of the literature on this topic, we refer the readers to the introductory parts of [2] and [3], but in the next paragraph we review some basic concepts and known facts about the nonlocal unitary operators and the controlled unitary operators.

Controlled unitary operators are a subclass of multipartite unitary operators. For example, the product of the local unitary operators on the local systems is the simplest controlled unitary. Such a unitary operator with *Schmidt rank* one is a local operator, also known as a product operator. Otherwise it is a *nonlocal* operator. Nonlocal unitaries can create quantum entanglement between distributed parties [4], and their equivalence has been studied under local operations and classical communication (LOCC) [5]. Without prior entanglement, nonlocal unitaries cannot be implemented by LOCC only, even if the probability is allowed to be close to zero [6]. To implement these tasks, it is desirable to have a simple type of nonlocal unitaries. The bipartite controlled unitary gates turn out to be such a type. They are of the general form $U = \sum_{j=1}^m P_j \otimes V_j$ acting on a bipartite Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$, where P_j are orthogonal projectors on \mathcal{H}_A and V_j are unitaries on \mathcal{H}_B . They can be implemented by a simple nonlocal protocol [7] using a maximally entangled state of Schmidt rank m . In this sense the implementation of controlled unitaries is operational. The bipartite controlled unitary gates are one of the few classes of bipartite unitaries for which their capacity to create entanglement between the parts is relatively well understood [8], and [9, 10] contain significant progress toward understanding their entanglement cost. Controlled unitaries also play an important role in quantum information theory, e.g. they are used in gate sets that are universal [11] for quantum computation [12], and they were also used in the creation of graph states (cluster states) [13], which find wide use in quantum communication protocols [14] and quantum computation.

In this paper, we study this problem via the Schmidt-rank-three bipartite and multipartite



or A,B swapped on right hand side

FIG. 1: Any bipartite unitary U of Schmidt rank three is locally equivalent to a controlled unitary, where the controlling side may be A or B . This is expressed as $U = (Q \otimes I)(\sum_{k=1}^{d_A} |k\rangle\langle k| \otimes V_k)(R \otimes I)$ or $U = (I \otimes Q)(\sum_{k=1}^{d_B} V_k \otimes |k\rangle\langle k|)(I \otimes R)$, where V_k , Q and R are local unitaries. The output systems A' and B' are assumed to be of the same size as A and B , respectively.

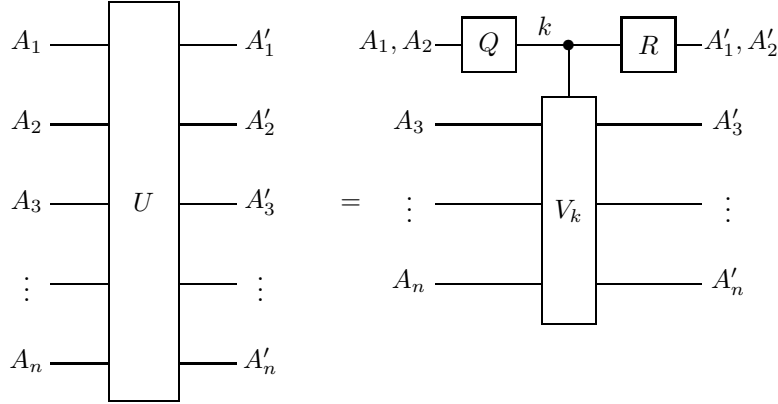


FIG. 2: Any n -partite unitary U of Schmidt rank three is locally equivalent to a controlled unitary by one system, or a unitary collectively controlled by two systems (but the systems are not arbitrary). The case that U is controlled by two systems is illustrated in the figure, and the case of one system acting as control is similar. The two controlling systems are denoted as A_1, A_2 . And $U = (Q \otimes I)(\sum_{k=1}^d |k\rangle\langle k| \otimes V_k)(R \otimes I)$, where Q and R are unitary operations on the space $\mathcal{H}_1 \otimes \mathcal{H}_2$ of dimension d , and V_k are unitary operations on $\mathcal{H}_3 \otimes \dots \otimes \mathcal{H}_n$. The output systems A'_1, \dots, A'_n are assumed to be of the same size as A_1, \dots, A_n , respectively.

unitary operators. We show that any Schmidt-rank-three bipartite unitary operator on $d_A \times d_B$ system is locally equivalent to a controlled unitary operator, see Theorem 11 and Fig. 1. The theorem is proved by developing novel tools from linear algebra in Sec. II A. Our results directly generalize most findings and applications in [3]. In particular, we show that the unitary can be implemented by LOCC and a maximally entangled state $|\Psi_r\rangle = \frac{1}{\sqrt{r}} \sum_{i=1}^r |ii\rangle$, where $r = \min\{d_A^2, d_B\}$ and $d_A \leq d_B$, see Lemma 22. As an application different from those in [3], we show that any multipartite unitary operator of Schmidt rank three can be controlled by one system or collectively controlled by two systems, regardless of the number of systems of this operator. This is illustrated in Fig. 2 and Theorem 18. The theorem is further strengthened in Corollary 19, by which we show that every Schmidt-rank-three multipartite unitary is controlled by the union of two systems (such two systems are considered as one combined system). By “collectively controlled by m systems” we mean that, the appointed m systems are regarded as one system which controls the multipartite unitary, and the unitary is not controlled by any k ($k \leq m - 1$) systems.

We also study the Schmidt-rank-three n -qubit unitary U . For any odd $n \geq 3$, we present examples of U that are collectively controlled by two systems, see Eqs. (21) and (28). For any even $n \geq 4$, U turns out to be a controlled unitary, see Proposition 21. We also introduce a connection between the controlled unitary and Schmidt rank in Lemma 24. The algebra tools we develop also reproduce the main result in [2], see Lemma 25.

The rest of this paper is organized as follows. In Sec. II we introduce the preliminary knowledge.

In Sec. III we prove our main result that any Schmidt-rank-three bipartite unitary is a controlled unitary. Next we propose a few applications of the main result in Sec. IV. We show that any Schmidt-rank-three multipartite unitary is either a controlled unitary, or collectively controlled by two systems. In particular, any Schmidt-rank-three n -qubit unitary with any even $n \geq 4$ is a controlled unitary. We also discuss the implication of our main result to the entanglement cost of bipartite unitaries, the connection between the Schmidt rank of a unitary and the Schmidt number of some related quantum states, and give a simple proof for that any Schmidt-rank-two bipartite unitary is a controlled unitary. Finally, we conclude in Sec. V.

II. PRELIMINARIES

Let $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ be the complex Hilbert space of a finite-dimensional bipartite quantum system of Alice and Bob. We denote by d_A, d_B the dimension of \mathcal{H}_A and \mathcal{H}_B , respectively. It is known that \mathcal{H} is spanned by the computational basis $|i, j\rangle$, where $i = 1, \dots, d_A$, and $j = 1, \dots, d_B$. We shall denote $I_k = \sum_{i=1}^k |i\rangle\langle i|$. For convenience, we denote $I_A = I_{d_A}$, $I_B = I_{d_B}$ and $I = I_{d_A d_B}$ as the identity operator on spaces $\mathcal{H}_A, \mathcal{H}_B$, and \mathcal{H} , respectively. Two bipartite unitary operators U, V on \mathcal{H} are *locally equivalent* when there are two product unitaries S_1, S_2 such that $U = S_1 V S_2$. We say that U is a *controlled unitary gate*, if U is locally equivalent to $\sum_{j=1}^{d_A} |j\rangle\langle j| \otimes U_j$ or $\sum_{j=1}^{d_B} V_j \otimes |j\rangle\langle j|$. To be specific, U is a controlled unitary from A or B side. Next, U has Schmidt rank n if there is a Schmidt decomposition (or expansion) $U = \sum_{j=1}^n A_j \otimes B_j$ where the $d_A \times d_A$ matrices A_1, \dots, A_n are linearly independent, and the $d_B \times d_B$ matrices B_1, \dots, B_n are also linearly independent. In particular, the zero matrix has Schmidt rank zero. We name the A (B) space of U as the space spanned by all A_j (B_j) that appear in a Schmidt decomposition of U . It is well defined in the sense that the space is independent of the specific choice of the Schmidt decomposition. For example, the identity operator I is the simplest controlled unitary and has Schmidt rank one.

Let us recall the concept of block-controlled unitary gate [3]. We split the space into a direct sum: $\mathcal{H}_A = \oplus_{i=1}^m \mathcal{H}_i$, $m > 1$, $\text{Dim } \mathcal{H}_i = m_i$, and $\mathcal{H}_i \perp \mathcal{H}_j$ for distinct $i, j = 1, \dots, m$. We say that U is a *block-controlled unitary (BCU) gate controlled from the A side*, if U is locally equivalent to $\sum_{i=1}^m \sum_{j,k=1}^{m_i} |u_{ij}\rangle\langle u_{ik}| \otimes V_{ijk}$ where $|u_{i,1}\rangle, \dots, |u_{i,m_i}\rangle$ is an orthonormal basis of \mathcal{H}_i . Note that the V_{ijk} are not necessarily unitary. For simplicity we denote the decomposition as $\oplus_A V_i$ where $V_i = \sum_{j,k=1}^{m_i} |u_{ij}\rangle\langle u_{ik}| \otimes U_{ijk}$, and we denote $|V_i|_A = m_i$. We have $U U^\dagger = \sum_{i=1}^m P_{\mathcal{H}_i} \otimes I_B = I$. In this paper we give an alternative and more easily accessible definition of BCU as follows. A unitary U is a BCU controlled from the A side if and only if $U = \sum_i |a_i\rangle\langle b_i| \otimes V_i + \sum_j |c_j\rangle\langle e_j| \otimes W_j$ where $\langle a_i|c_j\rangle = \langle b_i|e_j\rangle = 0$, $\forall i, j$. One may similarly define the BCU gate controlled from the B side. We shall use both definitions in the remaining part of this paper, and say U is a BCU when it is from either A or B side. By definition every controlled unitary with the condition $d_A d_B > 1$ is a BCU. As this condition is generically satisfied, we will simply state that every controlled unitary is a BCU.

Not every bipartite unitary is a BCU. For example, the SWAP gate $\frac{1}{2} \sum_{i=0}^3 \sigma_i \otimes \sigma_i$ acts on two-qubit space and has Schmidt rank 4. Here $\sigma_0 = I_2$, and

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (1)$$

are standard Pauli matrices. By definition, the SWAP gate is neither a controlled unitary nor a BCU. We will refer to $W \oplus_A X$ as *the direct sum of matrices W and X from the A side*, or A -direct sum of W and X . Here W, X respectively act on the subspaces $\mathcal{H}_i \otimes \mathcal{H}_B$, $i = 1, 2$, where $\mathcal{H}_1 \perp \mathcal{H}_2$. Indeed, both controlled unitaries and BCU are the direct sum of some blocks.

A. Preliminary results on linear algebra

We present a few preliminary lemmas based on linear algebra. They are useful for our main result Theorem 11, as well as the investigation of multipartite unitaries in Sec. IV.

Lemma 1 *Let A be a square matrix and $AA^\dagger = \sum_{i=1}^k c_i P_i$, where the c_i are distinct nonnegative real numbers, and the projectors P_i are pairwise orthogonal. Then*

- (i) *$A = (\sum_{i=1}^k c_i^{\frac{1}{2}} P_i) V$, where V is a unitary matrix.*
- (ii) *If furthermore A is normal, then $A = \oplus_{i=1}^k c_i^{\frac{1}{2}} U_i$, where the U_i is a unitary on the subspace of P_i .*
- (iii) *Let W, X be two unitary matrices and $W(\sum_{i=1}^k c_i P_i)X = \sum_{i=1}^k c_i P_i$. Then $W = \oplus_{i=1}^k W_i$ and $X = \oplus_{i=1}^k X_i$, where the W_i and X_i are two unitary matrices on the subspace of P_i , and $W_i = X_i^\dagger$ for all i such that c_i is nonzero.*
- (iv) *Let W, X be two unitary matrices and $WDX = D$, where D is a diagonal positive definite matrix. Then $W = X^\dagger$.*

Proof. (i) The assertion is known in matrix theory.

(ii) Since A is normal and $AA^\dagger = \sum_{i=1}^k c_i P_i$, we have $A = U(\sum_{i=1}^k c_i^{\frac{1}{2}} P'_i)U^\dagger$ where U is a unitary and P'_i is a diagonal unitary on the space of P_i . Hence $P'_i(P'_j)^\dagger = \delta_{ij}P_i = P_iP_j$. It follows from $AA^\dagger = \sum_{i=1}^k c_i P_i$ that U and $\sum_{i=1}^k c_i P_i$ commute. Since the c_i are pairwise different, we have $U = V_1 \oplus \dots \oplus V_k$, where the V_i is a unitary on the space of P_i . Letting $U_i = V_i P'_i V_i^\dagger$ for all i leads to the assertion.

(iii) Since $W(\sum_{i=1}^k c_i P_i)X = \sum_{i=1}^k c_i P_i$, we have $X^\dagger(\sum_{i=1}^k c_i P_i)W^\dagger = \sum_{i=1}^k c_i P_i$. Their products are

$$W\left(\sum_{i=1}^k c_i^2 P_i\right)W^\dagger = X^\dagger\left(\sum_{i=1}^k c_i^2 P_i\right)X = \sum_{i=1}^k c_i^2 P_i. \quad (2)$$

Since the c_i are nonnegative, real and pairwise different, so are the c_i^2 . Eq. (2) implies that $W = \oplus_{i=1}^k W_i$ and $X = \oplus_{i=1}^k X_i$, where the W_i and X_i are two unitary matrices on the subspace of P_i . Since $W(\sum_{i=1}^k c_i P_i)X = \sum_{i=1}^k c_i P_i$, we have $c_i W_i X_i = c_i P_i$ for any i . Thus $W_i = X_i^\dagger$ for all i such that c_i is nonzero. So assertion (iii) follows.

(iv) Since D is a diagonal positive definite matrix, there is a permutation matrix P such that $D = P(\sum_{i=1}^k c_i P_i)P^\dagger$. Since $WDX = D$, we have

$$P^\dagger W P \left(\sum_{i=1}^k c_i P_i \right) P^\dagger X P = \sum_{i=1}^k c_i P_i. \quad (3)$$

Since D is positive definite, (iii) implies that $P^\dagger W P = (P^\dagger X P)^\dagger$. Hence $W = X^\dagger$. This completes the proof. \square

Lemma 2 *Any space spanned by two linearly independent square matrices contains a nonzero singular matrix.*

Proof. Denote the two matrices as A and B . If the assertion does not hold, then A and B are both invertible. Let λ be an eigenvalue of $A^{-1}B$, we have $\det(-\lambda I_A + A^{-1}B) = 0$, hence $\det(-\lambda A + B) = 0$, meaning that $C := -\lambda A + B$ is singular. Since A and B are linearly independent, C is nonzero. This completes the proof. \square

Lemma 3 Let A_1, A_2 be two linearly independent square matrices. Let x_i, y_i be two positive numbers, z_i one complex number, such that $x_i y_i > |z_i|^2$ for $i = 1, 2$ and

$$\begin{aligned} x_1 A_1^\dagger A_1 + y_1 A_2^\dagger A_2 + z_1 A_1^\dagger A_2 + z_1^* A_2^\dagger A_1 &= I, \\ x_2 A_1 A_1^\dagger + y_2 A_2 A_2^\dagger + z_2 A_1 A_2^\dagger + z_2^* A_2 A_1^\dagger &= I. \end{aligned} \quad (4)$$

Then the following statements hold:

(i) There are two positive numbers a, b , and two linearly independent matrices B_1, B_2 in the span of A_1, A_2 such that

$$\begin{aligned} B_1^\dagger B_1 + B_2^\dagger B_2 &= I, \\ a B_1 B_1^\dagger + b B_2 B_2^\dagger &= I. \end{aligned} \quad (5)$$

(ii) If one of B_1 and B_2 is not proportional to a unitary, then $a = b = 1$.

(iii) B_1 and B_2 always have simultaneous singular value decomposition, i.e., there are unitary matrices V, W such that VB_1W and VB_2W both diagonal.

Proof. (i) Since $x_i y_i > |z_i|^2$ for $i = 1, 2$, then (4) implies that there are two linearly independent matrices $A_3 = (x_1 - \frac{|z_1|^2}{y_1})^{\frac{1}{2}} A_1$, and A_4 in the space $H = \text{span}\{A_1, A_2\}$ such that

$$\begin{aligned} A_3^\dagger A_3 + A_4^\dagger A_4 &= I, \\ x A_3 A_3^\dagger + y A_4 A_4^\dagger + z A_3 A_4^\dagger + z^* A_4 A_3^\dagger &= I, \end{aligned} \quad (6)$$

with two positive numbers x, y , one complex number $z = |z|e^{-i\varphi}$ and a real phase φ . It follows from (4) and $x_2 y_2 > |z_2|^2$ that $xy > |z|^2$. If $x = y$, then (6) implies that $a = x + |z|$, $b = x - |z|$, and $B_{1,2} = \frac{1}{\sqrt{2}} A_3 \pm \frac{1}{\sqrt{2}} e^{i\varphi} A_4$ in (5). Since $x > |z|$, we have $a, b > 0$. Since B_1, B_2 span H , the assertion follows. It suffices to assume $x \neq y$. Let

$$B_1 = \cos \theta A_3 + e^{i\varphi} \sin \theta A_4, \quad (7)$$

$$B_2 = \sin \theta A_3 - e^{i\varphi} \cos \theta A_4, \quad (8)$$

$$a = \frac{1}{2}(x + y + \text{sgn}(x - y)\sqrt{(x - y)^2 + 4|z|^2}), \quad (9)$$

$$b = \frac{1}{2}(x + y - \text{sgn}(x - y)\sqrt{(x - y)^2 + 4|z|^2}), \quad (10)$$

where $\theta = \frac{1}{2} \arctan \frac{2|z|}{x-y}$, and $\text{sgn}()$ is the sign function. One can easily verify that these expressions make (5) and (6) the same. It follows from (10) and $xy > |z|^2$ that $a, b > 0$. Since B_1, B_2 span H , the assertion follows.

(ii) Up to local unitaries on the l. h. s. of (5), we may assume that $B_1 = \sum_{i=1}^k c_i^{\frac{1}{2}} P_i$, where the c_i are nonnegative, real and $c_i > c_{i+1}$ for all i , and the projectors P_i are pairwise orthogonal. Eq. (5) implies that $B_2^\dagger B_2 = I - B_1^\dagger B_1$ and $B_2 B_2^\dagger = \frac{1}{b} I - \frac{a}{b} B_1 B_1^\dagger$. The r.h.s. of both equations are diagonal matrices whose diagonals are in the ascending order. Since $B_2 B_2^\dagger$ and $B_2^\dagger B_2$ are similar matrices, they have identical eigenvalues. We have $B_2 B_2^\dagger = B_2^\dagger B_2 = \sum_{i=1}^k (1 - c_i) P_i$. Since one of B_1 and B_2 is not proportional to a unitary, we have $k > 1$. Then Eq. (5) implies that $a = b = 1$.

(iii) From (ii), we have that either B_1, B_2 are both proportional to unitaries, or none of B_1, B_2 are proportional to unitaries but they satisfy Eq. (5) with $a = b = 1$. In the former case, up to unitaries before and after the operators B_1 and B_2 , we may assume $B_1 \propto I_B$, and B_2 is diagonal, hence B_1 and B_2 have simultaneous singular value decomposition. In the latter case, up to unitaries we may assume B_1 is a diagonal matrix, i.e., $B_1 = \sum_{i=1}^k c_i^{\frac{1}{2}} P_i$, where the c_i are nonnegative, real,

pairwise different, and the projectors P_i are pairwise orthogonal. From Eq. (5) with $a = b = 1$, we have $B_2 B_2^\dagger = B_2^\dagger B_2 = \sum_{i=1}^k (1 - c_i) P_i$. So B_2 is normal. It follows from Lemma 1 that $B_2 = \oplus_{i=1}^k (1 - c_i)^{\frac{1}{2}} U_i$, where the U_i is a unitary on the subspace of P_i , and can be diagonalized simultaneously with P_i . Hence in the latter case, B_1 and B_2 also have simultaneous singular value decomposition. This completes the proof. \square

Lemma 4 Suppose a bipartite operator $\sum_{j=1}^N A_j \otimes B_j$ has Schmidt rank $r \geq 0$, and

$$\delta_A := \text{Dim}(\text{span}\{A_j\}_{j=1}^N), \quad (11)$$

$$\delta_B := \text{Dim}(\text{span}\{B_j\}_{j=1}^N). \quad (12)$$

Then

- (i) $\delta_A + \delta_B \leq N + r$;
- (ii) $r \leq \min\{\delta_A, \delta_B\} \leq \max\{\delta_A, \delta_B\} \leq N$;
- (iii) If $\max\{\delta_A, \delta_B\} = N$, then $\min\{\delta_A, \delta_B\} = r$.

Proof. (i) The assertion is from [15].

(ii) It is sufficient to prove the first inequality. If $r > \min\{\delta_A, \delta_B\}$, then the Schmidt rank of the bipartite operator is smaller than r . It gives us a contradiction, so the assertion follows.

(iii) The assertion follows from the definition of Schmidt rank. This completes the proof. \square

The converse of (iii) is wrong. If $\min\{\delta_A, \delta_B\} = r$, then we have $\max\{\delta_A, \delta_B\} \leq N$.

The equivalence between a bipartite and controlled unitary has been widely studied recently [2, 3]. For the purpose in this paper, we provide more equivalent conditions of deciding whether a bipartite unitary is a controlled unitary.

Lemma 5 Let $U = \sum_j A_j \otimes B_j$ be a bipartite unitary and consider the following five assertions:

- (i) U is a controlled unitary from the A side;
- (ii) there are two orthonormal basis $\{|a_i\rangle\}$ and $\{|b_i\rangle\}$ of \mathcal{H}_A such that $U = \sum_i (|a_i\rangle\langle a_i| \otimes I_B) U (|b_i\rangle\langle b_i| \otimes I_B)$;
- (iii) for two arbitrary orthonormal basis $\{|c_i\rangle\}$ and $\{|e_j\rangle\}$ of \mathcal{H}_B , there are unitaries S and T on \mathcal{H}_A such that the operators $(S \otimes \langle c_i|) U (T \otimes |e_j\rangle)$ on \mathcal{H}_A , $\forall i, j$ are all diagonal;
- (iv) the matrices A_i have simultaneous singular value decomposition.
- (v) the operators $A_i A_j^\dagger$, $\forall i, j$ are all normal and commute with each other, and the operators $A_i^\dagger A_j$, $\forall i, j$ are all normal and commute with each other.

Then the first three assertions are equivalent. If the operators $\{B_j\}$ are linearly independent, then all five assertions are equivalent.

Proof. The relation (i) \rightarrow (ii), (iii) follows from the definition of controlled unitaries. Let us prove the relation (ii) \rightarrow (i). Suppose there are two orthonormal basis $\{|a_i\rangle\}$ and $\{|b_i\rangle\}$ of \mathcal{H}_A such that $U = \sum_i (|a_i\rangle\langle a_i| \otimes I_B) U (|b_i\rangle\langle b_i| \otimes I_B)$. We assume the decomposition $U = \sum_{i,j} |a_i\rangle\langle b_j| \otimes U_{ij}$, and obtain $U_{ij} = 0$ for any $i \neq j$. So U is a controlled unitary from the A side, and (ii) \rightarrow (i) holds.

Next let us prove the relation (iii) \rightarrow (i). Suppose for two arbitrary orthonormal basis $\{|c_i\rangle\}$ and $\{|e_j\rangle\}$ of \mathcal{H}_B , there are unitaries S and T on \mathcal{H}_A such that the operators $(S \otimes \langle c_i|) U (T \otimes |e_j\rangle)$ on \mathcal{H}_A , $\forall i, j$ are all diagonal. We can always have the decomposition $U = \sum_{i,j} U_{ij} \otimes |c_i\rangle\langle e_j|$ with some operators U_{ij} on \mathcal{H}_A . Then all matrices $S U_{ij} T$ are diagonal. By definition U is a controlled unitary from the A side, and (iii) \rightarrow (i) holds. So we have shown that the first three assertions are equivalent.

To prove the claim in the last sentence of the lemma, suppose the operators $\{B_j\}$ are linearly independent. The relation (iv) \rightarrow (i) follows from the definition of controlled unitaries (see also [2,

Lemma 2]). The relation $(v) \rightarrow (i)$ is from [3, Lemma 2]. We now show that $(i) \rightarrow (iv), (v)$. Up to a permutation of labels, the A space of U is spanned by the linearly independent matrices A_1, \dots, A_r . We have the Schmidt decomposition $U = \sum_{i=1}^r A_i \otimes B'_i$, where each B'_i is a linear combination of $\{B_j\}$. Since the operators $\{B_j\}$ are linearly independent, any A_i is in the A space of U , thus from the definition of controlled unitaries we have $(i) \rightarrow (iv)$. It follows from [3, Lemma 2] that $(i) \rightarrow (v)$ holds when $i, j = 1, \dots, r$ in assertion (v) . For any k, l , we have $A_k A_l^\dagger \in \text{span}\{A_i A_j^\dagger\}_{i,j=1,\dots,r}$ and $A_k^\dagger A_l \in \text{span}\{A_i^\dagger A_j\}_{i,j=1,\dots,r}$. It implies $(i) \rightarrow (v)$, and thus the equivalence between any two of the five assertions $(i) - (v)$. This completes the proof. \square

Note that the proof for $(iii) \rightarrow (i)$ is similar to proving the so-called classical and generalized classical states [16]. The former has zero quantum discord, so there is no quantum correlation in the classical states [1]. They are both a class of separable states lying near the quantum-classical boundary, in the sense that each party of such states can perfectly identify a locally held state without disturbing the global state. This is a task known as non-disruptive local state identification, which is related to the problem of unambiguous state discrimination [16]. The counterpart of this task for controlled unitaries has been presented as Lemma 5 (ii). The generalized classical states also allow for another quantum-information task of *local broadcasting* [17]. An N -partite quantum state $\rho^{(12\dots N)}$ allows for local broadcasting if there exists local maps $\Lambda^{(i)} : \mathcal{H}^{(i)} \rightarrow \mathcal{H}^{(i)} \otimes \mathcal{H}^{(i)}$ such that the state $\sigma^{(11'22'\dots NN')} = [\Lambda^{(1)} \otimes \dots \otimes \Lambda^{(N)}]\rho$ has reduced states $\sigma^{(12\dots N)} = \sigma^{(1'2'\dots N')} = \rho$. However so far there is no counterpart of local broadcasting for controlled unitaries. Below we present a result that applies to all bipartite operators.

Lemma 6 *The following statements hold:*

- (i) *The A space and the B space of a Schmidt-rank- r bipartite operator each contains $r - 1$ linearly independent singular operators.*
- (ii) *Suppose a Schmidt-rank- r bipartite unitary with Schmidt decomposition $\sum_{i=1}^r A_i \otimes B_i$ satisfies $B_i|a\rangle = 0$ for a nonzero vector $|a\rangle$, $i = 2, \dots, r$. Then the unitary is a BCU from the B side, and A_1 is proportional to a unitary matrix. That is, the A space of U contains a unitary matrix.*

Proof. (i) Suppose a Schmidt expansion of the Schmidt-rank- r bipartite unitary is $U = \sum_{j=1}^r A_j \otimes B_j$. From Lemma 2, there is a nonzero linear combination of A_1 and A_2 that is singular, denoted as A'_1 . Apparently A'_1 is in the A space of U . We can re-expand U using r linearly independent operators on the A side including A'_1 . Now the remaining $r - 1$ A -side operators in such expansion also contains a singular operator, again from Lemma 2. Denote such operator as A'_2 . The A'_2 is linearly independent from A'_1 , since the $r - 1$ A -side operators above together with A'_1 form a linearly independent set. We can re-expand U using r operators on the A side including A'_1 and A'_2 . This process can repeat until we find $r - 1$ linearly independent singular operators $A'_1, A'_2, \dots, A'_{r-1}$. Hence the A space of U contains $r - 1$ linearly independent singular operators. The proof is similar for the B space.

(ii) Let $U = \sum_{i=1}^r A_i \otimes B_i$. From $U^\dagger U = I$, we have $\sum_{i,j=1}^r A_i^\dagger A_j \otimes B_i^\dagger B_j = I$. Since $B_i|a\rangle = 0$ for a nonzero vector $|a\rangle$, $i = 2, \dots, r$, we have $(I_A \otimes \langle a|)U^\dagger U(I_A \otimes |a\rangle) = \langle a|B_1^\dagger B_1|a\rangle A_1^\dagger A_1 = I_A$. So A_1 is proportional to a unitary matrix.

It remains to prove that U is a BCU from the B side. Since $B_i|a\rangle = 0$ for $i \geq 2$, there exist two $d_B \times d_B$ unitaries V and W such that $VB_1W = \begin{pmatrix} B_{11} & 0 \\ B_{12} & B_{13} \end{pmatrix}$ and $VB_iW = \begin{pmatrix} B_{i1} & 0 \\ B_{i2} & 0 \end{pmatrix}$, $i \geq 2$, where B_{11} and B_{i1} are of size $(d_B - 1) \times (d_B - 1)$. Let $U' = (I_A \otimes V)U(I_A \otimes W)$, which is locally equivalent to U . Since U is unitary, U' is also unitary and the complex number B_{13} is nonzero.

Since $(U')^\dagger U' = I$, we have

$$\sum_{j=1}^r A_1^\dagger A_j \otimes B_{13}^* B_{j2} = 0. \quad (13)$$

We have proven that A_1 is proportional to a unitary and $B_{13} \neq 0$. Thus (13) implies $\sum_{j=1}^r A_j \otimes B_{j2} = 0$. Since $U = \sum_{j=1}^r A_j \otimes B_j$ has Schmidt rank r , the r matrices A_1, \dots, A_r are linearly independent. These arguments imply $B_{j2} = 0$ for all j . So

$$\begin{aligned} U' &= A_1 \otimes \begin{pmatrix} B_{11} & 0 \\ 0 & B_{13} \end{pmatrix} + \sum_{i=2}^r A_i \otimes \begin{pmatrix} B_{i1} & 0 \\ 0 & 0 \end{pmatrix} \\ &= \left(A_1 \otimes B_{13} |d_B\rangle\langle d_B| \right) + \left(\sum_{i=1}^r A_i \otimes B_{i1} \right). \end{aligned} \quad (14)$$

By definition U' is a BCU from the B side. Since U and U' are locally equivalent, U is also a BCU from the B side. This completes the proof. \square

III. SCHMIDT-RANK-THREE BIPARTITE UNITARIES

In this section we show that any Schmidt-rank-three bipartite unitary is a controlled unitary. This is the main result, as proved in Theorem 11. For this purpose, we present four preliminary lemmas 7, 8, 9, and 10. They characterize the properties of Schmidt-rank-three bipartite unitaries and some of them might be generalized to bipartite unitaries of higher Schmidt rank. The proof of these lemmas are intimately related to the linear algebra constructed in Sec. II A and the concepts in the preliminaries such as BCU. Although they are both preliminaries for Theorem 11, the lemmas in this section work for only Schmidt-rank-three bipartite unitaries.

Lemma 7 *The following two statements are equivalent:*

- (i) *any Schmidt-rank-three bipartite unitary is a controlled unitary;*
- (ii) *any Schmidt-rank-three bipartite unitary is a BCU.*

Proof. To prove the lemma, we first prove the following statement:

If a bipartite unitary U of Schmidt rank three is the direct sum from A side of two unitaries T_1, T_2 , and satisfies one of the following conditions:

- (a) *one of T_1, T_2 is a Schmidt-rank-three controlled unitary from B side;*
- (b) *both T_1, T_2 are controlled unitaries;*

then U is a controlled unitary.

The proof for the statement is as follows:

Suppose $U = T_1 \oplus_A T_2$, where T_1, T_2 are unitaries.

For condition (a): without loss of generality assume T_1 is controlled from the B side and has Schmidt rank three. From Lemma 5, the basis of three B side operators for T_1 can be simultaneously diagonalized under local unitaries. Since U is also of Schmidt rank three, the linear span of such three B side operators contains the B side operators in the Schmidt expansion of T_2 . Hence all B side operators of U are simultaneously diagonalized under local unitaries. From Lemma 5, U is a controlled unitary from the B side. So the assertion follows.

For condition (b): If T_1, T_2 are both controlled from the A side, then U is also a controlled unitary from the A side. Otherwise, it must be that one of the two controlled unitaries, say T_1 is controlled from the B side only. Then T_1 is of Schmidt rank at least 3, since unitaries with Schmidt rank not exceeding 2 are controlled from both sides [2]. Since U has Schmidt rank three, so is T_1 .

Thus condition (i) holds, and hence U is a controlled unitary from the B side. This completes the proof of the statement.

For the lemma, the implication (i) \rightarrow (ii) is obvious. To prove the implication (ii) \rightarrow (i), we present a method for proving that any Schmidt-rank-three bipartite unitary is a controlled unitary that involves induction over the dimensions d_A and d_B . The induction hypothesis is that any Schmidt-rank-three bipartite unitary on $k \times l$ ($k \geq 2, l \geq 2$) system is a controlled unitary, when either $k \leq d_A - 1, l \leq d_B$ or $k \leq d_A, l \leq d_B - 1$. The boundary case is that $k = 2$ or $l = 2$, and is proved in [3]. By condition (ii), the Schmidt-rank-three unitaries U on $d_A \times d_B$ system is always a BCU. We can always choose to divide U into two blocks only rather than many blocks, and use the induction hypothesis to get that each block is a controlled unitary, then the previously proved statement when condition (b) holds implies that the whole unitary is a controlled unitary. This proves the incremental case in the induction hypothesis when the dimensions are (d_A, d_B) . This completes the proof. \square

Lemma 8 *Consider a Schmidt-rank-three bipartite unitary operator whose A space is spanned by unitary matrices. Then the operator is $\sum_{i=1}^3 A_i \otimes B_i$, where $\{A_i\}$ are unitary and at least one of the B_i is non-invertible.*

Proof. Suppose the Schmidt-rank-three bipartite unitary is $U = \sum_{i=1}^3 X_i \otimes Y_i$ where $\{X_i\}$ are unitary. If one of $\{Y_i\}$ is non-invertible then the assertion follows. It suffices to consider that $\{Y_i\}$ are all invertible. There is a complex number x such that $B_1 = Y_1 - xY_2$ is non-invertible. We have $U = X_1 \otimes B_1 + (xX_1 + X_2) \otimes Y_2 + X_3 \otimes Y_3$. Let $|a\rangle$ be a state such that $B_1|a\rangle = 0$. Since $(I_A \otimes \langle a|)U^\dagger U(I_A \otimes |a\rangle) = I_A$, we have

$$\left((xX_1 + X_2) \otimes Y_2|a\rangle + X_3 \otimes Y_3|a\rangle \right)^\dagger \cdot \left((xX_1 + X_2) \otimes Y_2|a\rangle + X_3 \otimes Y_3|a\rangle \right) = I_A. \quad (15)$$

Because Y_2 and Y_3 are invertible, we have $Y_2|a\rangle \neq 0$ and $Y_3|a\rangle \neq 0$. Thus there is a complex number y such that $-yY_2|a\rangle + Y_3|a\rangle$ is orthogonal to $Y_2|a\rangle$. Since X_3 is unitary, Eq. (15) implies that $xX_1 + X_2 + yX_3$ is nonzero and proportional to a unitary. We have $U = X_1 \otimes B_1 + (xX_1 + X_2 + yX_3) \otimes Y_2 + X_3 \otimes (-yY_2 + Y_3)$. By assuming $X_1 = A_1$, the second and third products as $A_2 \otimes B_2$ and $A_3 \otimes B_3$, respectively, we obtain the assertion. This completes the proof. \square

Lemma 9 *Any Schmidt-rank-three non-BCU bipartite unitary cannot have one of its spaces spanned by unitary matrices.*

Proof. The proof is by contradiction. Assume there is a Schmidt-rank-three non-BCU bipartite unitary satisfying that one of its spaces is spanned by unitary matrices. Let U be such a Schmidt-rank-three non-BCU bipartite unitary whose A space is spanned by three unitary matrices. These three unitaries are not simultaneously diagonalizable, since otherwise U is a controlled unitary, contradicting with the non-BCU condition. From Lemma 8, we have $U = \sum_{j=1}^3 A_j \otimes B_j$, where A_j are all unitary and B_3 is non-invertible. Let B_3 be of rank $r \in [1, d_B - 1]$. Up to local unitaries on \mathcal{H}_B , we may assume that $B_3 = P \oplus 0_{d_B-r}$ is diagonal and P is a $r \times r$ invertible matrix. Let $B_i = \begin{pmatrix} B_{i1} & B_{i2} \\ B_{i3} & B_{i4} \end{pmatrix}$ for $i = 1, 2$, and B_{i1} is of size $r \times r$. If $B_{12} = B_{22} = 0$, then there are two complex numbers x, y such that $xB_{14} + yB_{24}$ is nonzero and singular. We re-expand the unitary as $U = A'_1 \otimes (xB_1 + yB_2) + A'_2 \otimes B'_2 + A_3 \otimes B_3$. Let $|a\rangle \in \text{span}\{|r+1\rangle, \dots, |d_B\rangle\}$ be a state such that $(xB_{14} + yB_{24})|a\rangle = 0$. Hence $(xB_1 + yB_2)|a\rangle = B_3|a\rangle = 0$. Lemma 6 (ii) implies that U is a BCU from the B side, a contradiction with the assumption. Below we assume that one of B_{12} and B_{22} is not zero.

Up to a unitary similarity transform on \mathcal{H}_A , we may assume that $A_1 = I_A$, $A_2 = D$, and the identical diagonal entries of D are adjacent. Let $D = e^{i\theta_1}P_1 + e^{i\theta_2}P_2 + \dots + e^{i\theta_k}P_k$, where $k \geq 2$, the projectors P_i are pairwise orthogonal, and $\theta_i \in (0, 2\pi)$ are pairwise different. We write A_3 as a partitioned matrix $A_3 = [V_{ij}]_{i,j=1,\dots,k}$, where the submatrix V_{ij} is of size $|P_i| \times |P_j|$, and the diagonal blocks V_{ii} are all upper-triangular. If the blocks V_{jm} are zero for all distinct integers j, m , then the unitarity of U implies that all V_{ii} are diagonal. U is a controlled unitary from the A side, it is a contradiction with the assumption that the A -side unitaries are not simultaneously diagonalizable. So there are two distinct integers j, m such that $V_{jm} \neq 0$. Since U is unitary, there is another integer n different from j , such that $V_{nj} \neq 0$. Let V'_{ii} be the same as V_{ii} , except that the diagonals of V'_{ii} are replaced by zeros. From $U^\dagger U = I$ we have

$$\begin{aligned} & I_A \otimes (B_1^\dagger B_1 + B_2^\dagger B_2 + B_3^\dagger B_3) + D \otimes B_1^\dagger B_2 \\ & + D^\dagger \otimes B_2^\dagger B_1 + A_3 \otimes B_1^\dagger B_3 + A_3^\dagger \otimes B_3^\dagger B_1 \\ & + D^\dagger A_3 \otimes B_2^\dagger B_3 + A_3^\dagger D \otimes B_3^\dagger B_2 = I. \end{aligned} \quad (16)$$

By considering the off-diagonal part of the A side operators in this equation, we obtain that the following partitioned matrix

$$\begin{aligned} & \begin{pmatrix} V'_{nn} & V_{nj} & V_{nm} \\ V_{jn} & V'_{jj} & V_{jm} \\ V_{mn} & V_{mj} & V'_{mm} \end{pmatrix} \otimes B_1^\dagger B_3 + \\ & \begin{pmatrix} (V'_{nn})^\dagger & V_{jn}^\dagger & V_{mn}^\dagger \\ V_{nj}^\dagger & (V'_{jj})^\dagger & V_{mj}^\dagger \\ V_{nm}^\dagger & V_{jm}^\dagger & (V'_{mm})^\dagger \end{pmatrix} \otimes B_3^\dagger B_1 + \\ & \begin{pmatrix} e^{-i\theta_n} V'_{nn} & e^{-i\theta_n} V_{nj} & e^{-i\theta_n} V_{nm} \\ e^{-i\theta_j} V_{jn} & e^{-i\theta_j} V'_{jj} & e^{-i\theta_j} V_{jm} \\ e^{-i\theta_m} V_{mn} & e^{-i\theta_m} V_{mj} & e^{-i\theta_m} V'_{mm} \end{pmatrix} \otimes B_2^\dagger B_3 + \\ & \begin{pmatrix} e^{i\theta_n} (V'_{nn})^\dagger & e^{i\theta_j} V_{jn}^\dagger & e^{i\theta_m} V_{mn}^\dagger \\ e^{i\theta_n} V_{nj}^\dagger & e^{i\theta_j} (V'_{jj})^\dagger & e^{i\theta_m} V_{mj}^\dagger \\ e^{i\theta_n} V_{nm}^\dagger & e^{i\theta_j} V_{jm}^\dagger & e^{i\theta_m} (V'_{mm})^\dagger \end{pmatrix} \otimes B_3^\dagger B_2 \end{aligned} \quad (17)$$

is zero. In particular if $m = n$, then each of the four blocks in the A side of (17) is replaced by

its upper left four blocks, say $\begin{pmatrix} V'_{nn} & V_{nj} & V_{nm} \\ V_{jn} & V'_{jj} & V_{jm} \\ V_{mn} & V_{mj} & V'_{mm} \end{pmatrix}$ is replaced by $\begin{pmatrix} V'_{nn} & V_{nj} \\ V_{jn} & V'_{jj} \end{pmatrix}$, etc. Since V_{jm} and

V_{nj} are nonzero and $\theta_j \in (0, 2\pi)$ are pairwise different, the space spanned by the four operators in the A side of (17) has dimension at least two. From (17) and Lemma 4, the space H spanned by the four operators $B_1^\dagger B_3$, $B_3^\dagger B_1$, $B_2^\dagger B_3$, and $B_3^\dagger B_2$ has dimension at most two. In the second paragraph we have shown that P is a $r \times r$ invertible matrix, and one of B_{12} and B_{22} is not zero. It implies $\dim H = 2$. By using this fact and also the block structure of the four B -side matrices, it can be determined that $B_1^\dagger B_3 \propto B_2^\dagger B_3$, and $B_3^\dagger B_1 \propto B_3^\dagger B_2$. Because $\dim H = 2$ and none of the four operators in A side of (17) is zero, neither are the operators $B_1^\dagger B_3$, $B_3^\dagger B_1$, $B_2^\dagger B_3$, and $B_3^\dagger B_2$. The two matrices $B_1^\dagger B_3$ and $B_3^\dagger B_1$ are linearly independent. Applying to (17) these facts and that V_{jm} and V_{nj} are nonzero, we have $\theta_j = \theta_n$. It is a contradiction with the fact that $\theta_j, \theta_n \in (0, 2\pi)$ are different. Therefore the assumption is wrong. This completes the proof. \square

Lemma 10 *Any Schmidt-rank-three non-BCU bipartite unitary $U = \sum_{j=1}^3 A_j \otimes B_j$ cannot satisfy the following condition:*

A_1 is the direct sum of a 2×2 upper left diagonal matrix and a $(d_A - 2) \times (d_A - 2)$ matrix, and A_2 is the direct sum of another upper left 2×2 diagonal matrix and another $(d_A - 2) \times (d_A - 2)$ matrix. The diagonal vectors of the two 2×2 matrices are linearly independent.

Proof. The proof is by contradiction. Assume the condition stated in the lemma holds. By replacing A_1, A_2 by a suitable linear combination of them and absorbing two global factors into B_1, B_2 , we may assume that the first two diagonal entries of A_1 and A_2 are 1, 0 and 0, 1, respectively. By replacing A_3 by a suitable linear combination of A_1, A_2 , and A_3 , we may assume that the first two diagonal entries of A_3 are zero. So the first rows of A_1 and A_3 are orthogonal, and the first columns of A_1 and A_3 are also orthogonal. Up to local unitaries on \mathcal{H}_B , we may assume that $B_3 = \sum_{i=1}^k c_i P_i$, where the projectors P_i are pairwise orthogonal, and the real and nonnegative c_i are pairwise different. Since $(\langle 1| \otimes I_B)U^\dagger U(|1\rangle \otimes I_B) = (\langle 1| \otimes I_B)UU^\dagger(|1\rangle \otimes I_B) = I_B$, we have

$$B_1^\dagger B_1 + w B_3^\dagger B_3 = B_1 B_1^\dagger + x B_3 B_3^\dagger = I_B, \quad (18)$$

with nonnegative and real numbers w, x . Since $(\langle 2| \otimes I_B)U^\dagger U(|2\rangle \otimes I_B) = (\langle 2| \otimes I_B)UU^\dagger(|2\rangle \otimes I_B) = I_B$, we have

$$B_2^\dagger B_2 + y B_3^\dagger B_3 = B_2 B_2^\dagger + z B_3 B_3^\dagger = I_B, \quad (19)$$

with nonnegative and real numbers y, z . If one of w, x, y, z is zero, then Lemma 6 implies that U is a BCU, a contradiction with the non-BCU condition in the lemma. Below we assume that none of w, x, y, z is zero. From $B_3 = \sum_{i=1}^k c_i P_i$, Eqs. (18) and (19), we have $w = x$ and $y = z$. Thus B_1, B_2 are normal. We have $B_1 B_1^\dagger = \sum_{i=1}^k (1 - w c_i^2) P_i$, and $B_2 B_2^\dagger = \sum_{i=1}^k (1 - y c_i^2) P_i$. Since $\{c_i\}$ are real, nonnegative, and pairwise different, so are $\{1 - w c_i^2\}$ and $\{1 - y c_i^2\}$, respectively. Then Lemma 1 implies that $B_1 = \oplus_{i=1}^k (1 - w c_i^2)^{\frac{1}{2}} U_i$ and $B_2 = \oplus_{i=1}^k (1 - y c_i^2)^{\frac{1}{2}} V_i$, where U_i, V_i are unitary matrices on the subspace of projector P_i and $U_i^\dagger U_i = V_i^\dagger V_i = P_i$ for all i . So U is the B-direct sum of the bipartite unitaries $X_i = A_1 \otimes (1 - w c_i^2)^{\frac{1}{2}} U_i + A_2 \otimes (1 - y c_i^2)^{\frac{1}{2}} V_i + A_3 \otimes c_i P_i$, $i = 1, \dots, k$. If $k > 1$, U is a BCU from the B side, a contradiction with the assumption in the lemma. Hence $k = 1$. Since U has Schmidt rank three, the B space of U is spanned by three unitary matrices U_1, V_1, I_B . This is a contradiction with Lemma 9, given that U is non-BCU. Hence the assumption is wrong. This completes the proof. \square

Theorem 11 *Any bipartite unitary of Schmidt rank three is a controlled unitary.*

Proof. Let $U = \sum_{j=1}^3 A_j \otimes B_j$ be a Schmidt-rank-three bipartite unitary. By Lemma 7, we only need to consider the cases that U is not a BCU, for the following reason: if we always get a contradiction for the non-BCU cases, for all dimensions d_A, d_B , then we would have proved that any Schmidt-rank-three bipartite unitary is a BCU, and from Lemma 7, any bipartite unitary of Schmidt rank three is a controlled unitary. Hence in the following we assume U is not a BCU. From Lemma 6(i) we may assume that A_1 is singular. Up to local unitaries on \mathcal{H}_A , we may assume $A_1|1\rangle = A_1^\dagger|1\rangle = 0$. Since $(\langle 1| \otimes I_B)U^\dagger U(|1\rangle \otimes I_B) = (\langle 1| \otimes I_B)UU^\dagger(|1\rangle \otimes I_B) = I_B$, we have

$$\begin{aligned} I_B &= x_1 B_2^\dagger B_2 + y_1 B_3^\dagger B_3 + z_1 B_2^\dagger B_3 + z_1^* B_3^\dagger B_2, \\ I_B &= x_2 B_2 B_2^\dagger + y_2 B_3 B_3^\dagger + z_2 B_2 B_3^\dagger + z_2^* B_3 B_2^\dagger, \end{aligned} \quad (20)$$

where x_i, y_i are non-negative and real numbers, z_i are complex numbers. They are given by $x_1 = \langle 1|A_2^\dagger A_2|1\rangle$, $y_1 = \langle 1|A_3^\dagger A_3|1\rangle$, $z_1 = \langle 1|A_2^\dagger A_3|1\rangle$, $x_2 = \langle 1|A_2 A_2^\dagger|1\rangle$, $y_2 = \langle 1|A_3 A_3^\dagger|1\rangle$, $z_2 = \langle 1|A_2 A_3^\dagger|1\rangle$. From these equations we get that the inequalities $x_i y_i \geq |z_i|^2$ hold for $i = 1, 2$. If one of the equalities hold then either $T|1\rangle = 0$ or $T^\dagger|1\rangle = 0$ for some $T \in \text{span}\{A_2, A_3\}$, then from Lemma 6(ii), U is a BCU, and we get a contradiction. So $x_i y_i > |z_i|^2$ for $i = 1, 2$. It follows from

Eq. (20) and Lemma 3 that there are two linearly independent matrices B_4, B_5 in $\text{span}\{B_2, B_3\}$ such that B_4, B_5 are simultaneously diagonalizable. Hence U is locally equivalent to the non-BCU bipartite unitary satisfying the condition stated in Lemma 10, but that lemma says the condition cannot be satisfied for non-BCU Schmidt-rank-three unitaries. This is a contradiction, hence we have shown a contradiction always exists for any dimensions d_A, d_B . Hence there is no non-BCU Schmidt-rank-three unitary in systems of any size, meaning that any Schmidt-rank-three bipartite unitary is a BCU. Then by Lemma 7, any bipartite unitary of Schmidt rank three is a controlled unitary. This completes the proof. \square

We can further decide the side from which U is controlled by Lemma 5, and the algorithm is described in [18].

IV. APPLICATIONS

In this section we propose a few applications of our results on general nonlocal unitary operators. To generalize our findings to multipartite case, we study Schmidt-rank-three multipartite unitary operators in Sec. IV A. We begin by defining the necessary terminologies, and then characterize the basic properties of multipartite unitaries in Lemma 12. We also present a few methods of constructing non-controlled Schmidt-rank three multipartite unitaries in Example 14. The main result of this section is that any multipartite unitary operator of Schmidt rank three can be controlled by one system or collectively controlled by two systems, regardless of the number of systems of this operator in Theorem 18. This is based on the preliminary lemmas 15, 16 and 17. The theorem is further strengthened in Corollary 19, by which we show that every Schmidt-rank-three multipartite unitary is controlled by the union of two systems.

Next, we study the Schmidt-rank-three n -qubit unitary U in Sec. IV B. We construct non-controlled U for any odd $n \geq 3$ in (28). The main result of this section is Proposition 21, which states that U for any even $n \geq 4$ is a controlled unitary. This is based on a preliminary lemma 20. In Sec. IV C, we show that any bipartite unitary operator of Schmidt rank three can be implemented by LOCC and a maximally entangled state $|\Psi_r\rangle = \frac{1}{\sqrt{r}} \sum_{i=1}^r |ii\rangle$, where $r = \min\{d_A^2, d_B\}$ and $d_A \leq d_B$, see Lemma 22. In Sec. IV D, we study the connection between the controlled unitary and Schmidt rank in Lemma 24. In Sec. IV E, we give an alternative proof of one of the main results in [2], using only the linear algebra developed in Sec. II. The main result is Lemma 25.

A. Schmidt-rank-three multipartite unitary operators

Multipartite quantum states, such as the Greenberger-Horne-Zeilinger (GHZ) states, W states [19] and graph states [20], are the fundamental ingredients of quantum information processing. Multipartite quantum states can be generated by using multipartite unitary operations and in particular, by using multipartite controlled unitary operations. Understanding the structure of multipartite unitary helps explore the problems such as the state classification, implementation, and the experimental violation of multipartite Bell-type inequalities [21]. In this section, we will investigate multipartite unitary operators of Schmidt rank three, by using the results developed for bipartite unitaries.

To investigate multipartite unitary operators, we generalize the definitions and terminologies for bipartite unitary operators. Let j_1, \dots, j_k be k distinct integers in the set $\{1, 2, \dots, n\}$, and $\bar{j}_1, \dots, \bar{j}_k$ the remaining $n - k$ distinct integers in the same set. We shall denote the k systems $\mathcal{A}_{j_1}, \dots, \mathcal{A}_{j_k}$ and the corresponding Hilbert space $\mathcal{H}_{j_1} \otimes \dots \otimes \mathcal{H}_{j_k}$ as $\mathcal{A}_{j_1, \dots, j_k}$ and $\mathcal{H}_{j_1, \dots, j_k}$, respectively. Let U be an n -partite unitary operator of the system $\mathcal{A}_{1, \dots, n}$ in the space $\mathcal{H}_{1, \dots, n}$ with $\text{Dim } \mathcal{H}_i = d_i$ for all i . We say that U has Schmidt rank r if $U = \sum_{i=1}^r A_{i,1} \otimes A_{i,2} \otimes \dots \otimes A_{i,n}$,

and U cannot be the sum of fewer product operators. U is a controlled unitary from the \mathcal{A}_j side when it is locally equivalent to $\sum_{j=1}^{d_j} |j\rangle\langle j| \otimes V_j$ where V_j is a unitary on the subspace $\mathcal{H}_{\overline{j}}$. We shall sometimes ignore the subscript j and just say that U is a controlled unitary. We say U is not a controlled unitary, or equivalently, U is a “non-controlled” unitary, when U is not controlled from any one system, but could be collectively controlled from two or more systems.

If we partition the system $\mathcal{A}_{1,\dots,n}$ into two larger systems $\mathcal{A}_{j_1,\dots,j_k}$ and $\mathcal{A}_{\overline{j_1,\dots,j_k}}$, then we can regard U as a bipartite unitary $U_{j_1,\dots,j_k;\overline{j_1,\dots,j_k}}$. Its Schmidt rank is defined as the dimension of the $\mathcal{A}_{j_1,\dots,j_k}$ space of U . It is evidently equal to the dimension of the $\mathcal{A}_{\overline{j_1,\dots,j_k}}$ space. Since U has Schmidt rank r , the Schmidt rank of $U_{j_1,\dots,j_k;\overline{j_1,\dots,j_k}}$ is between 1 and r . In particular, if it is equal to one, then U is the tensor product of two multipartite unitary operators on the subspaces $\mathcal{H}_{j_1,\dots,j_k}$ and $\mathcal{H}_{\overline{j_1,\dots,j_k}}$, respectively. Based on these terminologies and definitions, we characterize the properties of multipartite unitary as follows.

Lemma 12 *Let $U = \sum_{i=1}^r A_{i,1} \otimes A_{i,2} \otimes \dots \otimes A_{i,n}$ be an n -partite Schmidt-rank- r unitary operator. Then*

- (i) *For any integer $j \in [1, n]$, the r product operators $\{A_{i,1} \otimes \dots \otimes A_{i,j-1} \otimes A_{i,j+1} \otimes \dots \otimes A_{i,n}\}_{i=1,\dots,r}$ are linearly independent.*
- (ii) *U is a controlled unitary from the \mathcal{A}_j side if and only if the r operators $A_{1,j}, \dots, A_{r,j}$ have simultaneous singular value decomposition.*
- (iii) *U is a controlled unitary if there are integers j_1, \dots, j_k such that the r product operators $\{A_{i,j_1} \otimes \dots \otimes A_{i,j_k}\}_{i=1,\dots,r}$ span a 1-dimensional or 2-dimensional space.*

Proof. (i) Assume the assertion does not hold. Then one of these r product operators is a linear combination of the other $r-1$ product operators. By expanding U using such $r-1$ operators that act on the space $\mathcal{H}_{1,\dots,j-1,j+1,\dots,n}$, we obtain an expansion of U with $r-1$ terms which are product operators. Thus U has Schmidt rank not greater than $r-1$, a contradiction with the assumption. Hence the assertion holds.

(ii) From (i) and the fact that U has Schmidt rank r , the r product operators $\{A_{i,1} \otimes \dots \otimes A_{i,j-1} \otimes A_{i,j+1} \otimes \dots \otimes A_{i,n}\}_{i=1,\dots,r}$ are linearly independent. The assertion follows from Lemma 5 (iv).

(iii) Under the first condition, U is a controlled unitary from any system of $\mathcal{A}_{j_1,\dots,j_k}$. So the assertion holds. It suffices to prove the assertion under the second condition. Suppose the r product operators $\{A_{i,j_1} \otimes \dots \otimes A_{i,j_k}\}_{i=1,\dots,r}$ span a 2-dimensional space. Without loss of generality, let $A_{1,j_1} \otimes \dots \otimes A_{1,j_k}$ and $A_{2,j_1} \otimes \dots \otimes A_{2,j_k}$ be linearly independent. Thus $A_{l,j_1} \otimes \dots \otimes A_{l,j_k}$ with any $l > 2$ is their linear combination. By the same reason, there is at least one integer, say j_1 such that A_{1,j_1} and A_{2,j_1} are linearly independent. So A_{l,j_1} with any $l > 2$ is their linear combination. By partitioning the system $\mathcal{A}_{1,\dots,n}$ into \mathcal{A}_{j_1} and $\mathcal{A}_{\overline{j_1}}$, we obtain a Schmidt-rank-2 bipartite unitary $U_{j_1;\overline{j_1}}$. It is a controlled unitary from the \mathcal{A}_{j_1} side [2], and so is U . This completes the proof. \square

The “if” condition in Lemma 12 (iii) means that the $\mathcal{A}_{j_1,\dots,j_k}$ space has dimension one or two, but the converse is generally not true. So the corollary cannot be generalized to multipartite unitary of a larger Schmidt rank, as we show in the following example.

Example 13 Let V be the two-qubit SWAP gate, $W = (\sigma_0 \otimes \sigma_3)V(\sigma_0 \otimes \sigma_3)$, and $U = \frac{1}{\sqrt{2}}(V_{12} \otimes V_{34} + iW_{12} \otimes W_{34})$. One can easily verify that U is a four-qubit unitary operator of Schmidt rank bigger than three. The $\mathcal{A}_{j,k}$ space of U has dimension equal to or larger than two, and the equality holds when $(j, k) = (1, 2)$. Furthermore, the \mathcal{A}_j space with any j has dimension four. So U is not a controlled unitary. \square

One may develop more conditions equivalent to Lemma 12 (ii), by using the items in Lemma 5. It is known that any Schmidt-rank-2 multipartite unitary is a controlled unitary from any side

[2]. For $n = 2$, we have shown that all Schmidt-rank-three unitaries are controlled unitaries in [3] and Theorem 11. Below we present a few examples and methods of constructing non-controlled Schmidt-rank-three multipartite unitary.

Example 14 For $n = 3$, there has been a Schmidt-rank-three non-controlled three-qubit unitary [2]

$$U^{(3)} = \frac{1}{\sqrt{3}}(\sigma_0 \otimes \sigma_0 \otimes \sigma_0 + i\sigma_1 \otimes \sigma_1 \otimes \sigma_1 + i\sigma_3 \otimes \sigma_3 \otimes \sigma_3). \quad (21)$$

Below we construct two other sets of Schmidt-rank-three non-controlled unitaries of high dimensions. It is easy to verify that the matrix $U + \sigma_0 \otimes \sigma_0 \otimes (\sum_{i=3}^n |i\rangle\langle i|)$ is a $2 \times 2 \times n$ Schmidt-rank-three non-controlled unitary. Next, Let $V = U \otimes I_{\mathcal{A}'_1 \mathcal{A}'_2 \mathcal{A}'_3}$ be a tripartite unitary of the systems $\mathcal{B}_1, \mathcal{B}_2, \mathcal{B}_3$, where $\mathcal{B}_i = \mathcal{A}_i \mathcal{A}'_i$ and $I_{\mathcal{A}'_i}$ acts on the space $\mathbb{C}^{d'_i}$ for $i = 1, 2, 3$. Then V is a Schmidt-rank-three non-controlled unitary on the $2d'_1 \times 2d'_2 \times 2d'_3$ system. \square

In spite of these examples, we do not have a systematic method of constructing Schmidt-rank-three non-controlled unitaries.

Although the tripartite unitary $U^{(3)}$ is not a controlled unitary, the bipartite unitary $U^{(3)}_{j_1, j_2; \overline{j_1, j_2}}$ with any distinct j_1, j_2 is a controlled unitary by Theorem 11 and Lemma 12 (ii). That is, $U^{(3)}$ is collectively controlled by system \mathcal{A}_{12} . Next, the four-qubit unitary in Example 13 is a unitary collectively controlled by the system \mathcal{A}_{12} because of [2]. These facts turn out to be general. In Theorem 18 we will show that any Schmidt-rank-three multipartite unitary is collectively controlled by at most two systems. To prove this theorem, we present three preliminary lemmas.

Lemma 15 Let A_1, A_2, B_1, B_2 be square matrices, and A_1 singular. The following statements hold:

- (i) If B_2 is singular, then the span of $A_1 \otimes B_1$ and $A_2 \otimes B_2$ does not contain any invertible matrix.
- (ii) If $A_1 \otimes B_1 + A_2 \otimes B_2$ is unitary, then B_2 is proportional to a unitary matrix.

Proof. (i) Since A_1, B_2 are both singular, let $|a\rangle, |b\rangle$ be the states such that $A_1|a\rangle = B_2|b\rangle = 0$. Then any matrix V in the span of $A_1 \otimes B_1$ and $A_2 \otimes B_2$ satisfies $V|a, b\rangle = 0$. So V is singular and the assertion holds.

(ii) Let $U = A_1 \otimes B_1 + A_2 \otimes B_2$ be the unitary. Since A_1 is singular, let $|a\rangle$ be the state such that $A_1|a\rangle = 0$. Then $(\langle a| \otimes I_B)U^\dagger U(|a\rangle \otimes I_B) = I_B \propto B_2^\dagger B_2$. Hence B_2 is proportional to a unitary matrix. This completes the proof. \square

Lemma 16 Let $\sum_{i=1}^3 A_{i,1} \otimes A_{i,2} \otimes A_{i,3}$ be a Schmidt-rank-three tripartite unitary. The matrices in one of the two sets $\{A_{i,2}\}_{i=1,2,3}$ and $\{A_{i,3}\}_{i=1,2,3}$ have simultaneous singular value decomposition, if one of the following two conditions is satisfied:

- (i) there is a state $|b\rangle$ such that any two vectors in $\{A_{i,1}|b\rangle\}_{i=1,2,3}$ are nonzero and parallel.
- (ii) The matrices in $\{A_{i,1}\}_{i=1,2,3}$ have simultaneous singular value decomposition, and two matrices in $\{A_{i,1}\}_{i=1,2,3}$ are invertible.

Proof. (i) Let $U = \sum_{i=1}^3 A_{i,1} \otimes A_{i,2} \otimes A_{i,3}$. Since U is unitary, we have $(\langle b| \otimes I_{\mathcal{A}_{2,3}})U^\dagger U(|b\rangle \otimes I_{\mathcal{A}_{2,3}}) = I_{\mathcal{A}_{2,3}} = V^\dagger V$, where $V = \sum_{i=1}^3 x_i A_{i,2} \otimes A_{i,3}$ with nonzero complex numbers x_1, x_2, x_3 . So V is unitary. Since U has Schmidt rank three, so is V by Lemma 12 (i). Theorem 11 implies that V is a controlled unitary. The assertion follows from Lemma 5 (iv).

(ii) If U satisfies condition (ii), then it satisfies condition (i). So the assertion follows. This completes the proof. \square

Lemma 17 Let $U = \sum_{i=1}^3 A_{i,1} \otimes A_{i,2} \otimes \cdots \otimes A_{i,n}$ be an n -partite Schmidt-rank-3 unitary operator collectively controlled by $k \leq \lceil \frac{n}{2} \rceil$ systems of $\mathcal{A}_{1,\dots,n}$. Then

(i) for any integers $j_1, \dots, j_s \in [1, n]$ and $s \in [1, k-1]$, the $\mathcal{A}_{j_1, \dots, j_s}$ space of U is spanned by unitary matrices.

(ii) If $k \geq 2$, then

(ii.a) for any integer $j \in [1, n]$, the space $\text{span}\{A_{i,j}\}_{i=1}^3$ is spanned by three unitary matrices.

(ii.b) U is a Schmidt-rank-three bipartite unitary on any bipartite cut.

(iii) If $k \geq 3$, then

(iii.a) there are k distinct integers $l = j_1, \dots, j_k \in [1, n]$ such that for each l , the set $\{A_{i,l}\}_{i=1,2,3}$ contains a singular matrix.

(iii.b) Let $\{A_{i,l}\}_{i \in [1,3], l \in [1,n]}$ be the set of all singular matrices in $\{A_{i,j}\}$. Then the set $\{i_l\}$ consists of exactly two distinct integers in $\{1, 2, 3\}$. If $x \in \{1, 2, 3\} \setminus \{i_l\}$, then $A_{x,l}$ with any $l \in [1, n]$ is proportional to a unitary matrix.

(iii.c) Any matrix $A_{i,j}$ is normal.

Proof. (i) If the $\mathcal{A}_{j_1, \dots, j_s}$ space of U has dimension one or two, then it is spanned by unitary matrices [2]. Suppose the space has dimension three. Theorem 11 implies that $U_{j_1, \dots, j_s; \overline{j_1, \dots, j_s}}$ is a controlled unitary. Since $s < k$, the system $\mathcal{A}_{j_1, \dots, j_s}$ cannot control U . So the $\mathcal{A}_{j_1, \dots, j_s}$ space of U is spanned by unitary matrices. The assertion follows.

(ii) Let us prove (ii.a). Since $k \geq 2$, the unitary $U_{j_1; \overline{j_1}}$ is not a controlled unitary, for any j_1 . Hence from [2] and that U has Schmidt rank 3, $U_{j_1; \overline{j_1}}$ has Schmidt rank exactly 3. Thus the space $\text{span}\{A_{i,j_1}\}_{i=1}^3$ has dimension three and is the \mathcal{A}_{j_1} space of U . Therefore from (i), this space is spanned by three unitary matrices. Assertion (ii.a) holds.

To prove (ii.b), suppose there are integers j_1, \dots, j_k such that $U_{j_1, \dots, j_k; \overline{j_1, \dots, j_k}}$ has Schmidt rank one or two. Up to the exchange of subscripts, we may assume that the three product operators $\{A_{i,j_1} \otimes \cdots \otimes A_{i,j_k}\}_{i=1,2,3}$ span a 1-dimensional or 2-dimensional space. Then U is a controlled unitary, according to Lemma 12 (iii). It is a contradiction with the condition $k \geq 2$. Thus (ii.b) follows.

(iii) Since $k \geq 3$ implies $k \geq 2$, all assertions in (ii) apply to U . Assume there are at most $k-1$ integers, say $l = 1, \dots, k-1$ such that for each l , the set $\{A_{i,l}\}_{i=1,2,3}$ contains a singular matrix. It implies that any matrix in the set $\{A_{i,l'}\}_{i=1,2,3}$ with $l' > k-1$ is invertible. Since $k \geq 3$, (ii.b) implies that the bipartite unitaries $U_{1, \dots, k-2; 1, \dots, k-2}$ and $U_{1, \dots, k-1; 1, \dots, k-1}$ have both Schmidt rank three. They are controlled unitaries by Theorem 11. Since $\lceil \frac{n}{2} \rceil \geq k \geq 3$, they are controlled by the systems $\mathcal{A}_{k-1, \dots, n}$ and $\mathcal{A}_{k, \dots, n}$, respectively. Let $C_i = A_{i,k-1} \otimes B_i$, where $B_i = A_{i,k} \otimes \cdots \otimes A_{i,n}$ for $i = 1, 2, 3$. From Lemma 5 (v), the operators $B_i B_j^\dagger$ (resp. $C_i C_j^\dagger$), $\forall i, j$ are all normal and commute with each other, and the operators $B_i^\dagger B_j$ (resp. $C_i^\dagger C_j$), $\forall i, j$ are all normal and commute with each other. We have

$$[A_{i,k-1} A_{j,k-1}^\dagger \otimes B_i B_j^\dagger, A_{s,k-1} A_{t,k-1}^\dagger \otimes B_s B_t^\dagger] = 0, \quad (22)$$

$$[A_{i,k-1}^\dagger A_{j,k-1} \otimes B_i^\dagger B_j, A_{s,k-1}^\dagger A_{t,k-1} \otimes B_s^\dagger B_t] = 0, \quad (23)$$

for any $i, j, s, t \in [1, 3]$. Since any matrix in the set $\{A_{i,l'}\}_{i=1,2,3}$ with $l' > k-1$ is invertible, the matrices $\{B_i\}_{i=1,2,3}$ are all invertible. It is known that the product of any two invertible matrices is invertible. Using these facts, (22) and (23), we obtain that the operators $A_{i,k-1} A_{j,k-1}^\dagger$, $\forall i, j$ are all normal and commute with each other, and the operators $A_{i,k-1}^\dagger A_{j,k-1}$, $\forall i, j$ are all normal and commute with each other. So $\{A_{i,k-1}\}_{i=1,2,3}$ have simultaneous singular value decomposition.

Then U is a controlled unitary from \mathcal{A}_{k-1} side [18]. It is a contradiction with $k \geq 3$, so the assumption is wrong. The assertion (iii.a) follows.

Next we prove (iii.b). Evidently we have $\{i_l\} \subseteq \{1, 2, 3\}$. Suppose the two sets are equal. It means that there is a set of integers $S = \{l_1, l_2, l_3\} \in [1, n]$ such that A_{1,l_1} , A_{2,l_2} and A_{3,l_3} are all singular. From (iii.a), we can always find a set S in which two integers are different. That is, $|S| \geq 2$. If the inequality holds, let $|b_i\rangle$ be the states such that $\langle b_i | A_{i,l_i} = 0$ for $i = 1, 2, 3$. Then $(\langle b_1, b_2, b_3 | \otimes I_{\mathcal{A}_{4,\dots,n}}) U U^\dagger (|b_1, b_2, b_3\rangle \otimes I_{\mathcal{A}_{4,\dots,n}}) = 0$. This is a contradiction with the fact that U is unitary. So we have $|S| = 2$. Without loss of generality, we may assume $l_1 \neq l_2 = l_3$. Because of $k \geq 3$ and Theorem 11, the \mathcal{A}_{l_1, l_2} space of U is spanned by unitary matrices U_1, U_2, U_3 of Schmidt rank at most two. These matrices cannot have Schmidt rank one because of assertion (ii.a) and the fact that A_{1,l_1} , A_{2,l_2} and $A_{3,l_3} = A_{3,l_2}$ are singular. So U_1, U_2, U_3 all have Schmidt rank two. Next, (ii) implies that any U_i is the linear combination of two elements of $\{A_{i,l_1} \otimes A_{i,l_2}\}_{i=1,2,3}$. Note that A_{1,l_1} , A_{2,l_2} and $A_{3,l_3} = A_{3,l_2}$ are singular. From Lemma 15 (i), any U_i is the linear combination of $A_{2,l_1} \otimes A_{2,l_2}$ and $A_{3,l_1} \otimes A_{3,l_2}$. So the U_1, U_2, U_3 span a 2-dimensional space. It is a contradiction with the fact that they span the \mathcal{A}_{l_1, l_2} space of U , which has dimension three. Hence the two sets $\{i_l\}$ and $\{1, 2, 3\}$ are not equal. We obtain $\{i_l\} \subset \{1, 2, 3\}$.

Next, suppose $\{i_l\}$ consists of exactly one integer in $\{1, 2, 3\}$, say $i_l = 1$. It implies that any matrix $A_{i,l}$ with $i = 2, 3$ and $l = 1, \dots, n$ is invertible. Let

$$B_j = A_{j,3} \otimes \dots \otimes A_{j,n} \quad (24)$$

for $j = 1, 2, 3$. Assertion (ii.b) and Theorem 11 imply that $U_{12:\overline{12}}$ is a Schmidt-rank-three controlled unitary. It is controlled by the system $\mathcal{A}_{3,\dots,n}$, because of $k \geq 3$. And since $U_{12:\overline{12}} = \sum_{j=1}^3 A_{j,1} \otimes A_{j,2} \otimes B_j$ is a Schmidt decomposition across the bipartite cut $12 : \overline{12}$, the matrices $\{B_j\}_{j=1,2,3}$ have simultaneous singular value decomposition. Note that B_2, B_3 are both invertible. So from Lemma 16 (ii), one of the two sets $\{A_{j,1}\}_{j=1,2,3}$ and $\{A_{j,2}\}_{j=1,2,3}$ have simultaneous singular value decomposition. We have $k = 1$ and it is a contradiction with $k = 3$. Thus, the set $\{i_l\}$ consists of exactly two distinct integers in $\{1, 2, 3\}$. The first assertion of (iii.b) follows.

Without loss of generality, let $\{i_l\} = \{1, 2\}$. It implies that any matrix $A_{3,l}$ with $l = 1, \dots, n$ is invertible. By using (iii.a), we may assume that A_{11} and A_{22} are singular. Let $|c_1\rangle, |c_2\rangle$ be the states such that $A_{11}|c_1\rangle = A_{22}|c_2\rangle = 0$. Since U is unitary, we have $(\langle c_1, c_2 | \otimes I_{\mathcal{A}_{3,\dots,n}}) U^\dagger U (|c_1, c_2\rangle \otimes I_{\mathcal{A}_{3,\dots,n}}) = I_{\mathcal{A}_{3,\dots,n}} \propto A_{3,3}^\dagger A_{3,3} \otimes \dots \otimes A_{3,n}^\dagger A_{3,n}$. So $A_{3,3}, \dots, A_{3,n}$ are all proportional to unitary matrices. Next, since $k \geq 3$, the \mathcal{A}_{12} space of U is spanned by three unitary matrices of Schmidt rank at most two. Lemma 15 (i) implies that two of the three matrices are $b_{11}A_{11} \otimes A_{12} + b_{12}A_{31} \otimes A_{32}$ and $b_{21}A_{21} \otimes A_{22} + b_{22}A_{31} \otimes A_{32}$ with complex numbers $b_{11}, b_{12}, b_{21}, b_{22}$, where $b_{12}b_{22} \neq 0$, and at least one of b_{11} and b_{21} is nonzero. Since A_{11} and A_{22} are singular, Lemma 15 (ii) implies that A_{31} and A_{32} are both proportional to unitary matrices. We have shown that any A_{3l} with $l = 1, \dots, n$ is proportional to a unitary matrix. The second assertion of (iii.b) follows.

Lastly we prove (iii.c). We still use the definition of B_j in (24). An argument similar to those below (24) implies that $U = \sum_{j=1}^3 A_{j,1} \otimes A_{j,2} \otimes B_j$ is a Schmidt-rank-three unitary, and the matrices $\{B_j\}_{j=1,2,3}$ have simultaneous singular value decomposition. We choose $x = 3$ in the statement of (iii.b). Up to a local unitary on $\mathcal{H}_{1,\dots,n}$, we may assume $A_{31} = aI_{A_1}$ with some complex number a , $A_{32} = I_{A_2}$ and $B_3 = I_{\mathcal{A}_{3,\dots,n}}$. Up to another unitary on $\mathcal{H}_{\overline{12}}$, we may assume B_1, B_2 are both diagonal. Since $k \geq 3$, assertion (ii) implies that $U_{1:\overline{1}}$ is of Schmidt rank three, and it is controlled by the system $\mathcal{A}_{\overline{1}}$. Lemma 5 (v) implies

$$[A_{i,2}A_{j,2}^\dagger \otimes B_iB_j^\dagger, A_{s,2}A_{t,2}^\dagger \otimes B_sB_t^\dagger] = 0, \quad (25)$$

for any $i, j, s, t \in [1, 3]$. Let $i = t = 3$ and $j = s = 1, 2$. Then (25) becomes $[A_{j,2}^\dagger \otimes B_j^\dagger, A_{j,2} \otimes B_j] = 0$. Since both B_1, B_2 are diagonal, we have $[A_{j,2}^\dagger, A_{j,2}] = 0$. Thus $A_{j,2}$ is normal for $j = 1, 2, 3$. By

exchanging the system \mathcal{A}_2 and any other \mathcal{A}_i , one can similarly prove that $A_{j,i}$ is normal for $j = 1, 2, 3$. Thus the assertion (iii.c) holds. This completes the proof. \square

Assertion (iii.a) does not hold when $k = 2$. A counterexample is the three-qubit $U^{(3)}$ in (21). Now we are in a position to prove the main result of this section.

Theorem 18 *Every Schmidt-rank-three multipartite unitary is a controlled unitary, or is collectively controlled by two systems of $\mathcal{A}_{1,\dots,n}$.*

Proof. Assume the assertion does not hold. Let U be a Schmidt-rank-three n -partite unitary with $n \geq 2$, and U cannot be controlled by any two systems of $\mathcal{A}_{1,\dots,n}$. So all assertions in Lemma 17 apply to U . It follows from Theorem 11 that $n \geq 5$. Using Lemma 17 (iii) and a suitable local unitary, we may assume

$$U = A_1 \otimes A_2 \otimes \cdots \otimes A_n + D_1 \otimes D_2 \otimes \cdots \otimes D_n + aI_{\mathcal{A}_1} \otimes I_{\mathcal{A}_2} \otimes \cdots \otimes I_{\mathcal{A}_n}, \quad (26)$$

where any D_i is diagonal and the nonzero diagonal elements are in the upper left side of D_i , any A_i is normal, and a is a nonzero complex number. Since U cannot be controlled by any two systems of $\mathcal{A}_{1,\dots,n}$, Lemma 17 implies that $U_{12:\overline{12}}$ is a Schmidt-rank-three bipartite unitary. It is a controlled unitary controlled by the system $\mathcal{A}_{\overline{12}}$ by virtue of Theorem 11. Thus the three product matrices $B_1 = A_3 \otimes \cdots \otimes A_n$, $B_2 = D_3 \otimes \cdots \otimes D_n$, and $B_3 = I_{\mathcal{A}_3} \otimes \cdots \otimes I_{\mathcal{A}_n}$ have simultaneous singular value decomposition. Let W and V be unitaries on $\mathcal{H}_{3,\dots,n}$ such that $WB_iV = E_i$, $i = 1, 2, 3$, where E_i are all diagonal. In particular $E_3 = WB_3V = WV$ is a diagonal unitary. Hence $E_iE_3^\dagger = WB_iVE_3^\dagger$ are all diagonal. Note that $WB_3VE_3^\dagger = E_3E_3^\dagger = I$, and since $B_3 = I$, we have $W^\dagger = VE_3^\dagger$. Thus WB_iW^\dagger are all diagonal. If $(WB_1W^\dagger)(WB_2W^\dagger) \neq 0$, then there is a nonzero diagonal element in the same position of WB_1W^\dagger , WB_2W^\dagger and B_3 , respectively. Let this position be presented by the projector $|l\rangle\langle l|$. Then the fact $U^\dagger U = I$ implies $(I_{\mathcal{A}_{1,2}} \otimes \langle l|)U^\dagger U(I_{\mathcal{A}_{1,2}} \otimes |l\rangle) = I_{\mathcal{A}_{1,2}}$. So the \mathcal{A}_{12} space of U contains a Schmidt-rank-three unitary, and it is a contradiction with $k \geq 3$ and Theorem 11. So we have $(WB_1W^\dagger)(WB_2W^\dagger) = 0$, namely $B_1B_2 = 0$. It implies that there is an integer $i \in [3, n]$ such that $A_iD_i = 0$. Since $A_i \neq 0$, D_i is singular. We may assume $D_i = D \oplus 0$ where D is an $s \times s$ invertible diagonal matrix and $s < d_i$. The equation $A_iD_i = 0$ implies that $A_i = \begin{pmatrix} 0 & C_1 \\ 0 & C_2 \end{pmatrix}$, where C_1, C_2 are two blocks of size $s \times (d_i - s)$ and $(d_i - s) \times (d_i - s)$, respectively. Recall that A_i is normal. We have $C_1 = 0$, and C_2 is also normal. Hence, the three matrices A_i, D_i and $I_{\mathcal{A}_i}$ are simultaneously diagonalizable. Eq. (26) implies that U is a controlled unitary. It is a contradiction with the assumption. This completes the proof. \square

The theorem implies that a Schmidt-rank-three multipartite controlled unitary can be characterized through the collaboration of two systems. For example, we have seen that the Schmidt-rank-three 3-qubit unitary operation $U^{(3)}$ in (21) can be collectively controlled by any two systems of the operation. Consider the Schmidt-rank-three 5-qubit unitary $V = I_2 \otimes I_2 \otimes U^{(3)}$. Using Lemma 5 (v), one can show that V cannot be controlled by the system \mathcal{A}_{23} . Hence in spite of Theorem 18, a Schmidt-rank-three multipartite unitary may be not collectively controlled by two *random* systems.

Based on Theorem 18 we obtain the following result. We shall refer to “union” as the case that a multipartite unitary is controlled by the union of a few systems, and may also be controlled by fewer systems. This is different from “collectively control” defined on in Sec. I.

Corollary 19 *Every Schmidt-rank-three n -partite unitary with $n \geq 3$ is controlled by the union of two systems of $\mathcal{A}_{1,\dots,n}$. There exists a non-controlled Schmidt-rank-three tripartite unitary, i.e., it is collectively controlled by two systems of \mathcal{A}_{123} .*

Proof. The second assertion follows from (21). It suffices to prove the first assertion. Let U be a Schmidt-rank-three n -partite unitary with $n \geq 3$. Using Theorem 18, it suffices to prove the assertion when U is a controlled unitary. Without loss of generality, we may assume that U is controlled by system \mathcal{A}_1 . Lemma 12 (ii) implies that U is locally equivalent to $V = \sum_{i=1}^3 A_{i,1} \otimes A_{i,2} \otimes \cdots \otimes A_{i,n}$, where each $A_{i,1}$ is a diagonal matrix on \mathcal{H}_1 . By rewriting V we have

$$V = \sum_{i=1}^{d_1} |i\rangle\langle i| \otimes V_i, \quad (27)$$

where each $V_i \in \text{span}\{A_{i,2} \otimes \cdots \otimes A_{i,n}\}_{i=1,2,3}$ is a unitary on the space \mathcal{H}_T . Since the $\{A_{i,2} \otimes \cdots \otimes A_{i,n}\}_{i=1,2,3}$ are linearly independent, each V_i has Schmidt rank at most three. If some V_j has Schmidt rank three, then (a) V_j is a controlled unitary controlled by one system \mathcal{A}_k of $\mathcal{A}_{2,\dots,n}$, or (b) V_j has to be collectively controlled by two systems $\mathcal{A}_{l,m}$ of $\mathcal{A}_{2,\dots,n}$ by Theorem 18. In case (a), note that $V_j \in \text{span}\{A_{i,2} \otimes \cdots \otimes A_{i,n}\}_{i=1,2,3}$ has Schmidt rank three. Lemma 12 (ii) implies that the three matrices $A_{1,k}, A_{2,k}$ and $A_{3,k}$ have simultaneous singular value decomposition. So V is collectively controlled by the system $\mathcal{A}_{1,k}$, and the assertion follows. In case (b), Lemma 17 (ii) implies that V_j is a Schmidt-rank-three bipartite unitary on any bipartite cut. So the three product matrices $A_{i,l} \otimes A_{i,m}$, $i = 1, 2, 3$ have simultaneous singular value decomposition. So V is collectively controlled by the system $\mathcal{A}_{l,m}$, and the assertion follows.

It remains to prove the assertion when each V_i has Schmidt rank at most two. Ref. [2] implies that each V_i is a controlled unitary controlled by any system in $\mathcal{A}_{2,\dots,n}$. Let W_i, X_i be two unitary matrices on \mathcal{H}_2 such that the \mathcal{A}_2 space of $(W_i \otimes I_{\mathcal{A}_{3,\dots,n}})V_i(X_i \otimes I_{\mathcal{A}_{3,\dots,n}})$ is spanned by a diagonal basis. Let $W = \sum_{i=1}^{d_1} |i\rangle\langle i| \otimes W_i$ and $X = \sum_{i=1}^{d_1} |i\rangle\langle i| \otimes X_i$ be two unitary operators on \mathcal{H}_{12} . From (27), the \mathcal{A}_{12} space of $(W \otimes I_{\mathcal{A}_{3,\dots,n}})V(X \otimes I_{\mathcal{A}_{3,\dots,n}})$ is spanned by a diagonal basis. So V is collectively controlled by \mathcal{A}_{12} . This completes the proof. \square

To summarize, if a Schmidt-rank-three multipartite unitary U is a controlled unitary by a system say \mathcal{A}_1 , then it is also controlled by the union of two systems. Nevertheless, we do not know whether the two systems always contain \mathcal{A}_1 .

On the other hand, if U is collectively controlled by two systems, then it may be not collectively controlled by any one or any three systems. An example is when $U = U^{(n)}$ with any odd $n \geq 5$, see (28). On the other hand, $U^{(n)}$ is collectively controlled by any two systems of $\mathcal{A}_{1,\dots,n}$ by its symmetry and Theorem 18.

B. Schmidt-rank-three multiqubit unitary operators

Multiqubit controlled gates can be decomposed into certain elementary gates [11], and are more useful than the general multipartite unitaries. For example, controlled NOT (CNOT) gates are essential for the construction of universal quantum two-qubit gates used in quantum computing both theoretically and experimentally [11, 22, 23]. Recently CNOT gates have been proved to be implemented by trapped ions controlled by fully overlapping laser pulses [24]. Multiqubit graph and cluster states for one-way quantum computing are generated by controlled-Z gates [20]. Controlled phase gates have also been used to construct the mutually unbiased bases (MUBs) [25]. Motivated by these applications and results in previous sections, we explore the Schmidt-rank-three multiqubit unitaries.

It is known that a two-qubit unitary cannot have Schmidt rank three [26]. In (21), we have presented the Schmidt-rank-three non-controlled three-qubit unitary constructed in [2]. Indeed, we can show that the following Schmidt-rank-three n -qubit unitary

$$U^{(n)} = \frac{1}{\sqrt{3}}[(\sigma_0)^{\otimes n} + i(\sigma_1)^{\otimes n} + i(\sigma_3)^{\otimes n}] \quad (28)$$

with any odd $n \geq 3$ is not a controlled unitary. On the other hand, constructing a non-controlled Schmidt-rank-three 4-qubit unitary turns out to be impossible. For any even $n \geq 4$, we will show that the Schmidt-rank-three n -qubit unitary is a controlled unitary, see Proposition 21. This is the main result of this section. For this purpose we present the following preliminary lemma.

Lemma 20 Let $V = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & a & b & c \\ 0 & d & e & f \\ 0 & g & h & i \end{pmatrix}$ be a two-qubit operator. If V has rank one and Schmidt rank

one, then one of the following four conditions is satisfied:

- (i) $a = b = c = e = h = 0$, $di = fg$ and $d \neq 0$.
- (ii) $a = d = e = f = g = 0$, $bi = ch$ and $b \neq 0$.
- (iii) $a = b = c = d = g = 0$, $ei = fh$, and one of e, f, h is nonzero.
- (iv) $b = d = e = f = h = 0$ and $ai = cg$.

Proof. The proof is by straightforward computation. We investigate three cases: $d \neq 0$, $b \neq 0$ and $d = b = 0$. Since V has rank one and Schmidt rank one, the first and second cases imply (i) and (ii), respectively. In the third case, we study two subcases: one of e, f, h is nonzero, and they are all zero. They imply (iii) and (iv), respectively. This completes the proof. \square

Proposition 21 For any even integer $m \geq 4$, the Schmidt-rank-three m -qubit unitary is a controlled unitary.

Proof. Suppose the assertion is not true. It implies three items as the hypotheses. First, let n be the minimum even integer, such that $n \geq 4$ and

$$U = \sum_{i=1}^3 A_{i,1} \otimes A_{i,2} \otimes A_{i,3} \otimes \cdots \otimes A_{i,n} \quad (29)$$

is a non-controlled Schmidt-rank-three n -qubit unitary. So Lemma 17 (ii) applies to U . It implies the second hypothesis: the three 2×2 matrices $A_{1,j}, A_{2,j}, A_{3,j}$ with any $j \in [1, n]$ are linearly independent, and do not have simultaneous singular value decomposition. Third, U is a Schmidt-rank-three bipartite unitary on any bipartite cut. These hypotheses do not change if we switch any two systems of $\mathcal{A}_{123\dots n}$, or if we switch any two product operators $A_{i,1} \otimes A_{i,2} \otimes A_{i,3} \otimes \cdots \otimes A_{i,n}$ and $A_{j,1} \otimes A_{j,2} \otimes A_{j,3} \otimes \cdots \otimes A_{j,n}$ by relabeling the subscripts i, j . Since U is not a controlled unitary, Theorem 18 implies that U is collectively controlled by two systems of $\mathcal{A}_{123\dots n}$. We can switch the systems so that U is controlled by the system \mathcal{A}_{12} . The third hypothesis implies that the three matrices in the set $S = \{A_{i,1} \otimes A_{i,2}\}_{i=1,2,3}$ have simultaneous singular value decomposition.

We discuss in this paragraph three cases in terms of the ranks of the matrices in S , and will discuss the remaining fourth case in the next paragraph. First, if all matrices in S have rank one, then $UU^\dagger \neq I$. It is a contradiction with the first hypothesis that U is unitary. So one matrix in S has rank at least two. Next, if two matrices in S are invertible (with rank four), then (29) implies that there are two states $|a\rangle, |b\rangle \in \mathcal{H}_{12}$, and nonzero complex numbers c_1, c_2, c_3 , such that $(\langle a| \otimes I_{\mathcal{A}_{12}})U = \langle b| \otimes U'$ where $U' = \sum_{i=1}^3 c_i A_{i,3} \otimes \cdots \otimes A_{i,n}$. Since U is unitary, U' is a $(n-2)$ -qubit unitary. The third hypothesis implies that U' has Schmidt rank three by Lemma 12 (i). Since U is not a controlled unitary, neither is U' . Since $n \geq 4$, we obtain a contradiction with the first hypothesis that n is minimum. Thus two matrices in S are singular. Third, if there is a matrix of rank two in S , then up to the relabeling of subscripts and the switch of systems \mathcal{A}_1 and \mathcal{A}_2 , we may assume such matrix is $A_{1,1} \otimes A_{1,2}$, and it satisfies $\text{rank } A_{1,1} = 1$ and $\text{rank } A_{1,2} = 2$. Using a suitable product unitary on \mathcal{H}_{12} and absorbing a suitable factor into $A_{1,3}$, we may assume

$A_{1,1} = \text{diag}(1, 0)$ and $A_{1,2} = \text{diag}(1, c)$ with some positive number c . Note that the matrices in S have simultaneous singular value decomposition. Let W, X be two unitary matrices on \mathcal{H}_{12} such that $W(A_{i,1} \otimes A_{i,2})X$ is diagonal for $i = 1, 2, 3$. In particular, we may choose W, X such that $W(A_{1,1} \otimes A_{1,2})X = A_{1,1} \otimes A_{1,2}$. Since $A_{1,1} \otimes A_{1,2} = \text{diag}(1, c, 0, 0)$ and $c > 0$, Lemma 1 (iii) implies that W and X are both the direct sum of two 2×2 unitary matrices. Using this fact and noting that $W(A_{i,1} \otimes A_{i,2})X$ is diagonal for $i = 2, 3$, we obtain that $A_{i,1} \otimes A_{i,2}$ is the direct sum of two 2×2 matrices. Thus $A_{2,1}$ and $A_{3,1}$ are both diagonal. Since $A_{1,1} = \text{diag}(1, 0)$, U is a controlled unitary. This is a contradiction with the first hypothesis. So any matrix in S does not have rank two.

The three cases in the last paragraph imply that the three matrices in S have to respectively have rank one, one and four. Up to a relabeling of subscripts, we may assume

$$\begin{aligned} \text{rank } A_{1,j} &= \text{rank } A_{2,j} = 1, \\ \text{rank } A_{3,j} &= 2, \end{aligned} \tag{30}$$

with $j = 1, 2$. Up to a product unitary on \mathcal{H}_{12} , we may assume

$$A_{1,1} = A_{1,2} = \text{diag}(1, 0). \tag{31}$$

Note that U is controlled by \mathcal{A}_{12} . Let W_1, X_1 be two unitaries on \mathcal{H}_{12} such that

$$W_1(A_{1,1} \otimes A_{1,2})X_1 = A_{1,1} \otimes A_{1,2}, \tag{32}$$

and $W_1(A_{i,1} \otimes A_{i,2})X_1$ with $i = 2, 3$ are still diagonal. Eqs. (31), (32), and Lemma 1 (iii) imply that W_1 and X_1 are both the direct sum of integer 1 and a 3×3 unitary matrices. Since $W_1(A_{3,1} \otimes A_{3,2})X_1$ is diagonal, $A_{3,1} \otimes A_{3,2}$ is the direct sum of a complex number and a 3×3 matrix B_1 . Since $A_{3,1} \otimes A_{3,2}$ is invertible, B_1 is diagonal. So $A_{3,1}$ and $A_{3,2}$ are both diagonal. Up to a diagonal product unitary on \mathcal{H}_{12} , we may assume that $A_{3,1}$ and $A_{3,2}$ are both positive definite without changing $A_{1,1}$ and $A_{1,2}$ in (31). Note that U is still a controlled unitary controlled by \mathcal{A}_{12} . From (31) and Lemma 1 (iii), there exist two unitaries

$$W' = 1 \oplus W_2, \quad X' = 1 \oplus X_2 \tag{33}$$

on \mathcal{H}_{12} such that

$$\begin{aligned} W'(A_{1,1} \otimes A_{1,2})X' &= A_{1,1} \otimes A_{1,2}, \\ W'(A_{3,1} \otimes A_{3,2})X' &= A_{3,1} \otimes A_{3,2}, \end{aligned} \tag{34}$$

and $W'(A_{2,1} \otimes A_{2,2})X'$ is diagonal. Thus $A_{2,1} \otimes A_{2,2}$ is the direct sum of a complex number x and a 3×3 matrix B_2 . The second hypothesis implies that $A_{2,1} \otimes A_{2,2}$ is not parallel to $A_{1,1} \otimes A_{1,2}$. These facts, (30) and (33) imply $x = 0$. Thus $A_{2,1} \otimes A_{2,2}$ becomes the matrix V in Lemma 20. It satisfies one of the four conditions (i-iv) in Lemma 20. From (31) and the paragraph below (32), the four matrices $A_{1,1}, A_{3,1}, A_{1,2}$ and $A_{3,2}$ are all diagonal. Since U is not a controlled unitary, conditions (iii) and (iv) in Lemma 20 are excluded. Next, either condition (i) or (ii) in Lemma 20 implies that $A_{2,1} \otimes A_{2,2}$ is not normal. Since $W'(A_{2,1} \otimes A_{2,2})X'$ is diagonal, we have $W' \neq (X')^\dagger$. Since $A_{3,1} \otimes A_{3,2}$ is diagonal positive definite, we have a contradiction because of (34) and Lemma 1 (iv).

We have excluded all possible cases of the matrices in S . So the hypothesis is wrong, and the assertion holds. This completes the proof. \square

We claim that a nontrivial Schmidt-rank-three n -qubit unitary exists for every $n \geq 3$, where “nontrivial” means not the tensor product of a one-qubit unitary and a Schmidt-rank-three $(n-1)$ -qubit unitary. If n is odd then the claim follows from (28). For even n , let $V^{(n-1)} = (U^{(n-1)})^\dagger$

where the latter is defined in (28). Then $|1\rangle\langle 1| \otimes U^{(n-1)} + |2\rangle\langle 2| \otimes V^{(n-1)}$ is a Schmidt-rank-three n -qubit unitary. So the claim follows.

Proposition 21 implies that the Schmidt-rank-three n -qubit unitaries with odd and even n have different control properties. The reason that makes the difference might be from the mathematical structure of multiqubit unitaries, but a decisive proof is not known yet.

C. Entanglement cost of implementing a bipartite unitary

The following lemma generalizes [3, Lemma 9]. It follows simply from a few protocols of implementation and Theorem 11, as explained after the lemma.

Lemma 22 *Let $d_A \leq d_B$. Any bipartite unitary of Schmidt rank three can be implemented by using LOCC and the maximally entangled state $|\Psi_k\rangle$, where $k = \min\{d_A^2, d_B\}$.*

The d_A^2 term is from using teleportation [27] twice: Alice teleports her input system to Bob, and Bob does the unitary locally, and teleports back the part of the output system belonging to Alice to her. This requires two maximally entangled states $|\Psi_{d_A}\rangle$ ($d_A \leq d_B$), which contains $2\log_2 d_A$ ebits [7].

The d_B term is from the protocol for controlled unitaries in ref. [7], which uses a maximally entangled state of Schmidt rank equal to the number of terms in the expression of the unitary in the controlled form.

From this lemma, $\log_2 d_B$ ebits is an upper bound of the amount of entanglement needed to implement a bipartite unitary of Schmidt rank three. As discussed in [3], this upper bound can be saturated for some unitary with $d_A = 2$, $d_B = 3$.

It is still an open question whether there is a Schmidt-rank-three unitary that needs more than $\log_2 3$ ebits to exactly implement using LOCC. This is a question about the lower bound of entanglement cost of unitaries, and some known results are in Soeda *et al* [9] and Stahlke *et al* [10]. These results suggest the interesting case to look at is when the resource state has Schmidt rank greater than that of the unitary, but still with relatively small entanglement.

On the probabilistic implementation of unitaries of small Schmidt rank, the protocol involving gate-teleportation that implements some types of two-qubit or two-qudit unitaries in [28] can be generalized to a protocol that probabilistically implements an arbitrary unitary acting on a $(d_A \times d_B)$ -dimensional space, by using the generalized Bell-state measurements and removing the final corrections. This would implement any Schmidt-rank- r unitary with probability $1/(d_A d_B)^2$ using a maximally entangled state of Schmidt rank r , but in the cases of failure, it is hard to recover the desired unitary via local corrections.

D. Connection with the Schmidt number

The Schmidt number of a bipartite quantum state is firstly introduced in [29]. It becomes the standard Schmidt rank when the state is pure. The Schmidt number is an entanglement monotone under LOCC. Recently, a device independent Schmidt rank witness for bipartite pure states has been proposed by using the Hardy paradox [30]. So the Schmidt rank is to some degree an observable quantity, and it is well known that it has various applications in quantum information. Similar statements can be said for the Schmidt number. In this subsection we explore the relation between the Schmidt number and controlled unitaries. For the convenience of readers, we review the definition from [31].

Definition 23 Given the density matrix ρ of a bipartite system and all its possible decompositions in terms of pure states, namely $\rho = \sum_i p_i |\psi_i^{r_i}\rangle\langle\psi_i^{r_i}|$, where r_i denotes the Schmidt rank of $|\psi_i^{r_i}\rangle$, the Schmidt number of ρ is defined as $\min\{\max_i\{r_i\}\}$ where the minimum is taken over all decompositions.

For example, the separable state has Schmidt number one in terms of the definition. Since projectors are extremal in the set of normalized quantum states (trace-one positive semidefinite matrices), the Schmidt number of a pure state is equal to its Schmidt rank. Below we study how the Schmidt number of the output state of a bipartite unitary is related to the Schmidt rank of the unitary, when the input state is restricted to be a separable state. We have not obtained an exact relationship, but some partial results are presented below.

Observation. For any $r \geq 1$, all diagonal bipartite unitaries of Schmidt rank r satisfy that there is a pure product input state such that the corresponding output state has Schmidt rank r . The input state can be chosen to be $|+\rangle_A |+\rangle_B$, where $|+\rangle_A := \frac{1}{\sqrt{d_A}} \sum_{j=1}^{d_A} |j\rangle$, and $|+\rangle_B := \frac{1}{\sqrt{d_B}} \sum_{j=1}^{d_B} |j\rangle$.

Lemma 24 Suppose a bipartite unitary is of Schmidt rank r , and it acts on a separable input state.

- (i) The Schmidt number of the output state is equal to or smaller than r .
- (ii) The equality is always achievable by some suitable input state when ancillas of sufficient size are allowed as part of the extended input. In particular, when $r \leq 3$, the controlling party does not need any ancilla.
- (iii) When ancillas are not allowed, the equality is achieved by some suitable input state (dependent on the unitary) for any bipartite unitary of Schmidt rank $r \leq 2$, and not achieved for some bipartite unitary of Schmidt rank r where r is any given integer greater than 2.

Proof. (i) Let $U = \sum_{j=1}^r A_j \otimes B_j$ be a Schmidt-rank- r bipartite unitary. Suppose the separable input state is $\rho = \sum_i |\alpha_i\rangle\langle\alpha_i| \otimes |\beta_i\rangle\langle\beta_i|$. For each pure-state component $|\alpha_i\rangle\langle\alpha_i| \otimes |\beta_i\rangle\langle\beta_i|$, the corresponding output is $\sum_{j=1}^r A_j |\alpha_i\rangle \otimes B_j |\beta_i\rangle$, so it is of Schmidt rank not greater than r . By the definition of the Schmidt number, the overall output state has Schmidt number not greater than r . This conclusion holds regardless of whether ancillas are allowed for the input state, since the tensor product of U with identity operators on the ancillas still has Schmidt rank r . This proves (i).

(ii) If we are allowed to add ancillas \bar{A} and \bar{B} with sizes equal to that of A and B , respectively, then there is an input state $\frac{1}{\sqrt{d_A d_B}} \sum_{j=1}^{d_A} |j\rangle_A |j\rangle_{\bar{A}} \otimes \sum_{k=1}^{d_B} |k\rangle_B |k\rangle_{\bar{B}}$, such that the output state on $A\bar{A}B\bar{B}$ has Schmidt rank r across the $A\bar{A} : B\bar{B}$ cut, equal to the Schmidt rank of U . This proves the first part of (ii). For the second part, from Theorem 11 and [2], the unitary is a controlled unitary, so up to local unitaries and a possible swap of the A, B systems, the unitary is of the form $U = \sum_{j=1}^n |j\rangle\langle j| \otimes V_j$, where $n \geq r$, and V_j ($1 \leq j \leq n$) are unitaries, with r of them being linearly independent. Choose the input state to be $\frac{1}{\sqrt{d_A d_B}} \sum_{j=1}^{d_A} |j\rangle_A \otimes \sum_{k=1}^{d_B} |k\rangle_B |k\rangle_{\bar{B}}$, then the output state on $AB\bar{B}$ has Schmidt rank r across the $A : B\bar{B}$ cut, equal to the Schmidt rank of U . The effect of the local unitaries is to change the form of the input state above, but does not affect the size of the possible ancillas. This proves the second part of (ii).

(iii) In the following we assume ancillas are not allowed. The equality can obviously be achieved when $r = 1$. From [2], all bipartite unitaries of Schmidt rank 2 is locally equivalent to a diagonal unitary, thus from the Observation above, there is a product pure input state with the output state having Schmidt rank 2. In the case $r = 3$, U may be a controlled unitary on a $d_A \times 2$ system, then the maximum Schmidt number of the output state is 2, which is less than the Schmidt rank of the unitary. In the case $r = 4$, let U be the SWAP gate on two qubits, then the Schmidt number of the output state is always 1 for any separable input state. For $r > 4$, similar examples of unitaries with $\min\{d_A, d_B\} < r$ can be constructed so that the maximum Schmidt number of the output is

not greater than $\min\{d_A, d_B\}$ and thus less than r , when the input is separable. This completes the proof. \square

From the proof above, we see that for the question of whether the equality is achievable, the ancillas become important since addition of ancillas increase the dimensions of the local Hilbert spaces which are upper bounds for the Schmidt number of the output state.

Define the Schmidt rank of a multipartite pure state to be the minimum number of pure product states that sum to the given state. By defining the Schmidt number of a multipartite mixed state based on it, similar to Definition 23, we can consider the generalizations of the results above to the multipartite case. The ‘‘Observation’’ and Lemma 24 (i) can be straightforwardly generalized to the multipartite case, but Lemma 24 (ii)(iii) may need some modifications in generalization, and we leave it for future study.

E. Bipartite unitaries studied in Ref. [2]

The Schmidt-rank-two multipartite unitary operators have been thoroughly studied in [2]. Apart from the usefulness mentioned before, they are also useful for other quantum technology. For example, the unitary $|0\rangle\langle 0| \otimes (I_2)^{\otimes n} + |1\rangle\langle 1| \otimes (\sigma_1)^{\otimes n}$ can amplify a single spin by set of ancillary spins [32, Eq. (1)]. So it is meaningful to understand the Schmidt-rank-two unitaries from another point of view. In this subsection, we give an alternative proof of one of the main results in [2], using only the linear algebra in Sec. II.

Lemma 25 *Any bipartite unitary of Schmidt rank two is a controlled unitary controlled from either side, and is a diagonal unitary up to local unitaries.*

Proof. Let $U = \sum_{j=1}^2 A_j \otimes B_j$ be a Schmidt-rank-2 bipartite unitary. From Lemma 6 (i) we may assume that A_1 is singular. Up to local unitaries on \mathcal{H}_A , we may assume $A_1|1\rangle = 0$. Since $(\langle 1| \otimes I_B)U^\dagger U(|1\rangle \otimes I_B) = I_B$, we have

$$I_B = xB_2^\dagger B_2, \quad (35)$$

where x is a positive real number. Hence B_2 is proportional to a unitary. There is a complex number z such that the linear combination $A'_2 = zA_1 + A_2$ satisfies $\text{Tr}(A_2^\dagger A_1) = 0$, hence $U = A_1 \otimes B'_1 + A'_2 \otimes B_2$, where $B'_1 = B_1 - zB_2$. The operators B'_1 and B_2 are linearly independent. By considering $U^\dagger U = I$ and taking the partial trace over the A side, we have

$$I_B = sB_1'^\dagger B'_1 + tB_2^\dagger B_2, \quad (36)$$

where $s > 0$, $t > 0$. Hence from Eq. (35), we have that B'_1 is proportional to a unitary. By absorbing factors into the A-side operators A_1 and A'_2 , we have that both B'_1 and B_2 are unitaries. Up to local unitaries on \mathcal{H}_B , we may assume $B'_1 = I$ and B_2 is a diagonal unitary. Both operators are diagonal, thus U is controlled from the B side.

The argument above also works with the A and B sides swapped. Hence U is a controlled unitary, controlled from either side. Up to local unitaries, $U = \sum_{j=1}^{d_A} |j\rangle\langle j| \otimes C_j$, where C_j are unitaries on \mathcal{H}_B . Then we have $C_j \in \text{span}\{C_g, C_h\}$ for two distinct integers g, h in $\{1, 2, \dots, d_A\}$, and up to local unitaries on \mathcal{H}_B , we have that $C_g = I_B$, and C_h is a diagonal unitary, hence all C_j are diagonal, therefore U is a diagonal unitary up to local unitaries. This completes the proof. \square

V. CONCLUSIONS

We have shown that any bipartite unitary operator of Schmidt rank three is locally equivalent to a controlled unitary. We have shown that LOCC and the $r \times r$ maximally entangled state of $r = \min\{d_A^2, d_B\}$ (under the assumption that $d_A \leq d_B$) are sufficient to implement such operators. We further show that any multipartite unitary operator of Schmidt rank three is a controlled unitary, or collectively controlled by two systems, regardless of the number of systems of this operator. We further show that the Schmidt-rank-three n -qubit unitary with any even $n \geq 4$ is a controlled unitary. We also have found a connection between the Schmidt number and controlled unitaries, in terms of the separable inputs and ancillas. Using the methods in this paper we have retrieved a main result of [2] in a different way.

There are many interesting open problems arising in this paper. It is expected that the technique and results developed here could be useful for characterizing nonlocal unitaries of larger Schmidt rank. Next, we have sort of characterized the Schmidt-rank-three multiqubit unitary in terms of $U^{(n)}$ and Proposition 21. It is unknown whether multiqubit unitaries of higher Schmidt rank can be similarly characterized. This is related to an unproved intuition that the Schmidt-rank-three multiqubit unitary might have a simpler structure than the general Schmidt-rank-three multipartite unitary. Another interesting problem is to construct a deeper connection between the nonlocal unitaries and Schmidt number of a bipartite or multipartite mixed state, extending the results in Sec. IV D. We also do not know the entanglement cost of implementing a Schmidt-rank-three multipartite unitary operation. Finally, although we have shown that any Schmidt-rank-three multipartite unitary is collectively controlled by at most two systems, an efficient method for finding out the two systems is still lacking.

ACKNOWLEDGMENTS

We thank Scott Cohen, Joseph Fitzsimons and Yingkai Ouyang for useful discussions or helpful comments. This material is based on research funded by the Singapore National Research Foundation under NRF Grant No. NRF-NRFF2013-01.

-
- [1] Harold Ollivier and Wojciech H. Zurek. Quantum discord: A measure of the quantumness of correlations. *Phys. Rev. Lett.*, 88:017901, Dec 2001.
 - [2] Scott M. Cohen and Li Yu. All unitaries having operator Schmidt rank 2 are controlled unitaries. *Phys. Rev. A*, 87:022329, Feb 2013.
 - [3] Lin Chen and Li Yu. Nonlocal and controlled unitary operators of Schmidt rank three. *Phys. Rev. A*, 89:062326, Jun 2014.
 - [4] J. Eisert, K. Jacobs, P. Papadopoulos, and M. B. Plenio. Optimal local implementation of nonlocal quantum gates. *Phys. Rev. A*, 62:052317, Oct 2000.
 - [5] W. Dür and J. I. Cirac. Equivalence classes of non-local unitary operations. *Quantum Information & Computation*, 2(3):240–254, 2002.
 - [6] Martin B. Plenio and Vlatko Vedral. Teleportation, entanglement and thermodynamics in the quantum world. *Contemporary Physics*, 39(6):431–446, 1998.
 - [7] Li Yu, Robert B. Griffiths, and Scott M. Cohen. Efficient implementation of bipartite nonlocal unitary gates using prior entanglement and classical communication. *Phys. Rev. A*, 81:062315, Jun 2010.
 - [8] Xiaoguang Wang, Barry C. Sanders, and Dominic W. Berry. Entangling power and operator entanglement in qudit systems. *Phys. Rev. A*, 67:042323, Apr 2003.

- [9] Akihito Soeda, Peter S. Turner, and Mio Muraio. Entanglement cost of implementing controlled-unitary operations. *Phys. Rev. Lett.*, 107:180501, Oct 2011.
- [10] Dan Stahlke and Robert B. Griffiths. Entanglement requirements for implementing bipartite unitary operations. *Phys. Rev. A*, 84:032316, Sep 2011.
- [11] Adriano Barenco, Charles H. Bennett, Richard Cleve, David P. DiVincenzo, Norman Margolus, Peter Shor, Tycho Sleator, John A. Smolin, and Harald Weinfurter. Elementary gates for quantum computation. *Phys. Rev. A*, 52:3457–3467, Nov 1995.
- [12] M. A. Nielsen and I. L. Chuang. *Quantum Computation and Quantum Information*. Cambridge University Press, Cambridge, 2000.
- [13] Dirk Schlingemann. Logical network implementation for cluster states and graph codes. *Quantum Information & Computation*, 3:431, 2003.
- [14] Charles H. Bennett and Gilles Brassard. Quantum cryptography: public key distribution and coin tossing. In *Proceedings of IEEE International Conference on Computers, Systems and Signal Processing, Bangalore, India*, pages 175–179. IEEE, New York, 1984.
- [15] Scott M. Cohen. Conditions for uniqueness of product representations for separable quantum channels and separable quantum states. *J. Math. Phys.*, 55(6):062202, 2014.
- [16] Lin Chen, Eric Chitambar, Kavan Modi, and Giovanni Vacanti. Detecting multipartite classical states and their resemblances. *Phys. Rev. A*, 83:020101, Feb 2011.
- [17] Marco Piani, Pawel Horodecki, and Ryszard Horodecki. No-local-broadcasting theorem for multipartite quantum correlations. *Phys. Rev. Lett.*, 100:090502, Mar 2008.
- [18] Takanori Maehara and Kazuo Murota. Simultaneous singular value decomposition. *Linear Algebra and its Applications*, 435(1):106 – 116, 2011.
- [19] W. Dür, G. Vidal, and J. I. Cirac. Three qubits can be entangled in two inequivalent ways. *Phys. Rev. A*, 62:062314, 2000.
- [20] Hans J. Briegel and Robert Raussendorf. Persistent entanglement in arrays of interacting particles. *Phys. Rev. Lett.*, 86:910–913, Jan 2001.
- [21] P. Lanyon, B. M. Zwerger, P. Jurcevic, C. Hempel, W. Dür, J. Briegel, H. R. Blatt, and F. Roos, C. Experimental violation of multipartite bell inequalities with trapped ions. *Phys. Rev. Lett.*, 112:100403, Mar 2014.
- [22] Tycho Sleator and Harald Weinfurter. Realizable universal quantum logic gates. *Phys. Rev. Lett.*, 74:4087–4090, May 1995.
- [23] J. I. Cirac and P. Zoller. A scalable quantum computer with ions in an array of microtraps. *Nature*, 404:579–581, April 2000.
- [24] Vladimir S. Malinovskiy, Ignacio R. Sola, and Jiri Vala. Phase-controlled two-qubit quantum gates. *Phys. Rev. A*, 89:032301, Mar 2014.
- [25] M Wiesniak, T Paterek, and A Zeilinger. Entanglement in mutually unbiased bases. *New Journal of Physics*, 13(5):053047, 2011.
- [26] Michael A. Nielsen, Christopher M. Dawson, Jennifer L. Dodd, Alexei Gilchrist, Duncan Mortimer, Tobias J. Osborne, Michael J. Bremner, Aram W. Harrow, and Andrew Hines. Quantum dynamics as a physical resource. *Phys. Rev. A*, 67:052301, May 2003.
- [27] Charles H. Bennett, Gilles Brassard, Claude Crépeau, Richard Jozsa, Asher Peres, and William K. Wootters. Teleporting an unknown quantum state via dual classical and einstein-podolsky-rosen channels. *Phys. Rev. Lett.*, 70:1895–1899, Mar 1993.
- [28] F. V. Mendes and R. V. Ramos. On the role of the basis of measurement in quantum gate teleportation. <http://arxiv.org/abs/1307.4750>, July 2013.
- [29] Barbara M. Terhal and Paweł Horodecki. Schmidt number for density matrices. *Phys. Rev. A*, 61:040301, Mar 2000.
- [30] Amit Mukherjee, Arup Roy, Some S. Bhattacharya, Subhadipa Das, Md, and Manik Banik. Device independent Schmidt rank witness by using Hardy paradox. <http://arxiv.org/abs/1407.2146>, July 2014.
- [31] Anna Sanpera, Dagmar Bruß, and Maciej Lewenstein. Schmidt-number witnesses and bound entanglement. *Phys. Rev. A*, 63:050301, Apr 2001.
- [32] Tom Close, Femi Fadugba, Simon C. Benjamin, Joseph Fitzsimons, and Brendon W. Lovett. Rapid and robust spin state amplification. *Phys. Rev. Lett.*, 106:167204, Apr 2011.